Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

A Sequential One-pot Approach to 1,2,4,5-Tetrasubstituted-2*H*-imidazole Synthesis from Disubstituted Alkynes:

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General information:

All chemicals were purchased form best grade in commercially available and are used without further purification. All solvents were purchased as HPLC grade and used without any purification or distillation. Analytical thin layer chromatography was performed on aluminum plate coated with silica gel (Merck). Gravity column chromatography was performed using 100-200 mesh silica gel and mixtures of hexane-ethyl acetate were used for elution. Visualization was accomplished using ultraviolet light (254 nm) and chemical staining with acidic potassium permanganate solution and Iodine.

Melting points was determined using "Mel-Temp" melting point apparatus and were uncorrected.

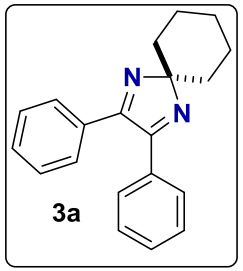
Proton nuclear magnetic resonance (^{1}H NMR) and Carbon nuclear magnetic resonance (^{13}C NMR) spectra's were recorded using a Varian (400 MHz) spectrometer. All spectra were recorded at ambient temperature (298 K). Chemical shifts (δ) are quoted in ppm relative to residual solvent ($CDCl_3$: δ = 7.26 ppm for ^{1}H and δ = 77.0 for 13C; $(CD_3)_2SO$: δ = 2.50 ppm for ^{1}H). Coupling constants (*J*) are corrected and quoted to the nearest 0.1 Hz. The following abbreviations are used to indicate the multiplicity of the signals: s = singlet; d = doublet; t = triplet; q = quartet; m = multiplet; bs = broad singlet; dt = doublet of triplet; td = triplet of doublet.

High resolution mass spectra (HRMS) were measured on a Micromass Q-TOF spectrometer using EI (electron impact, 70 eV) at the Joint Center for High valued Instruments, NSYS University, Kaohsiung, Taiwan.

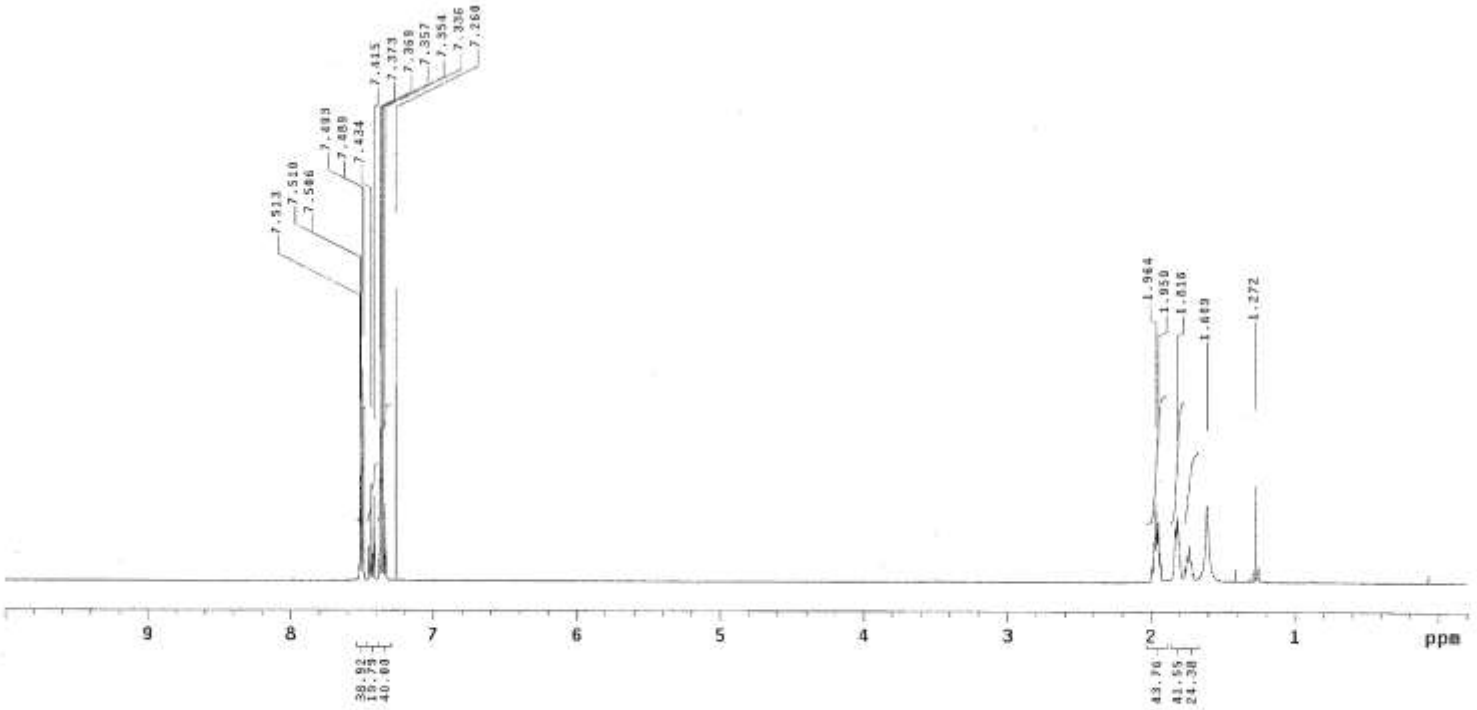
BPPSCY

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Dec 1 2014
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



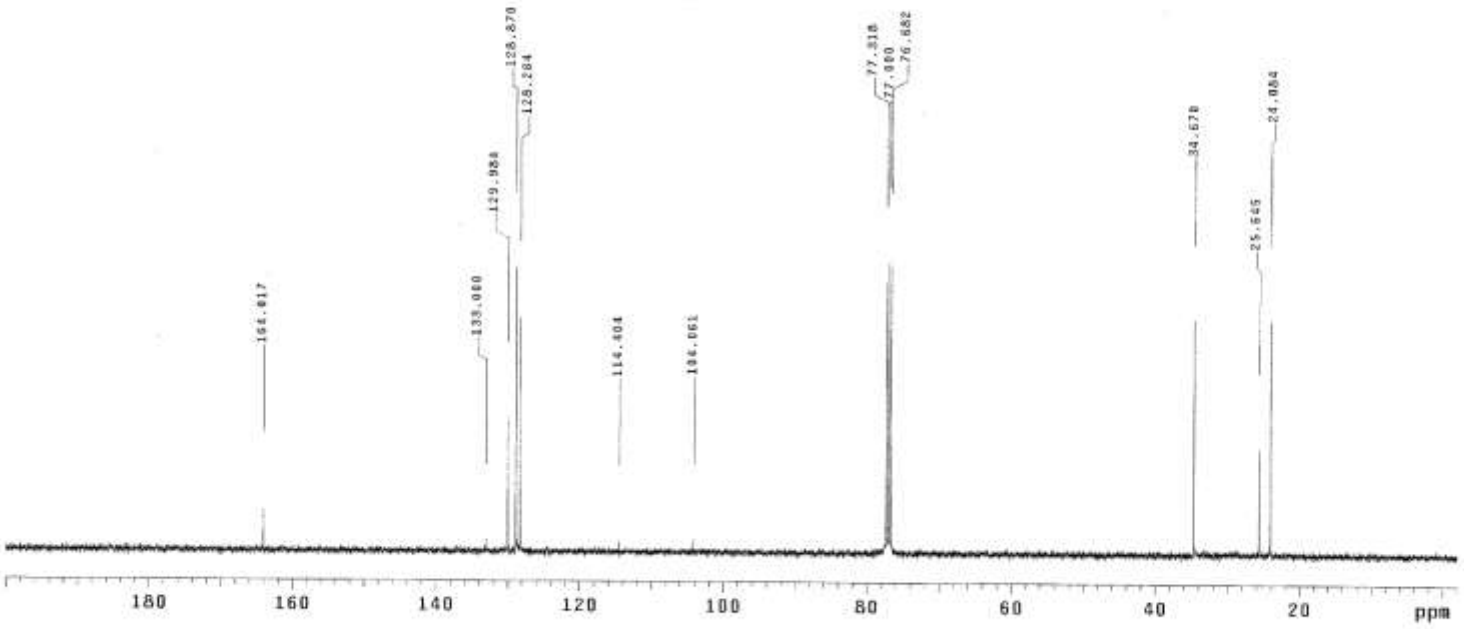
3a

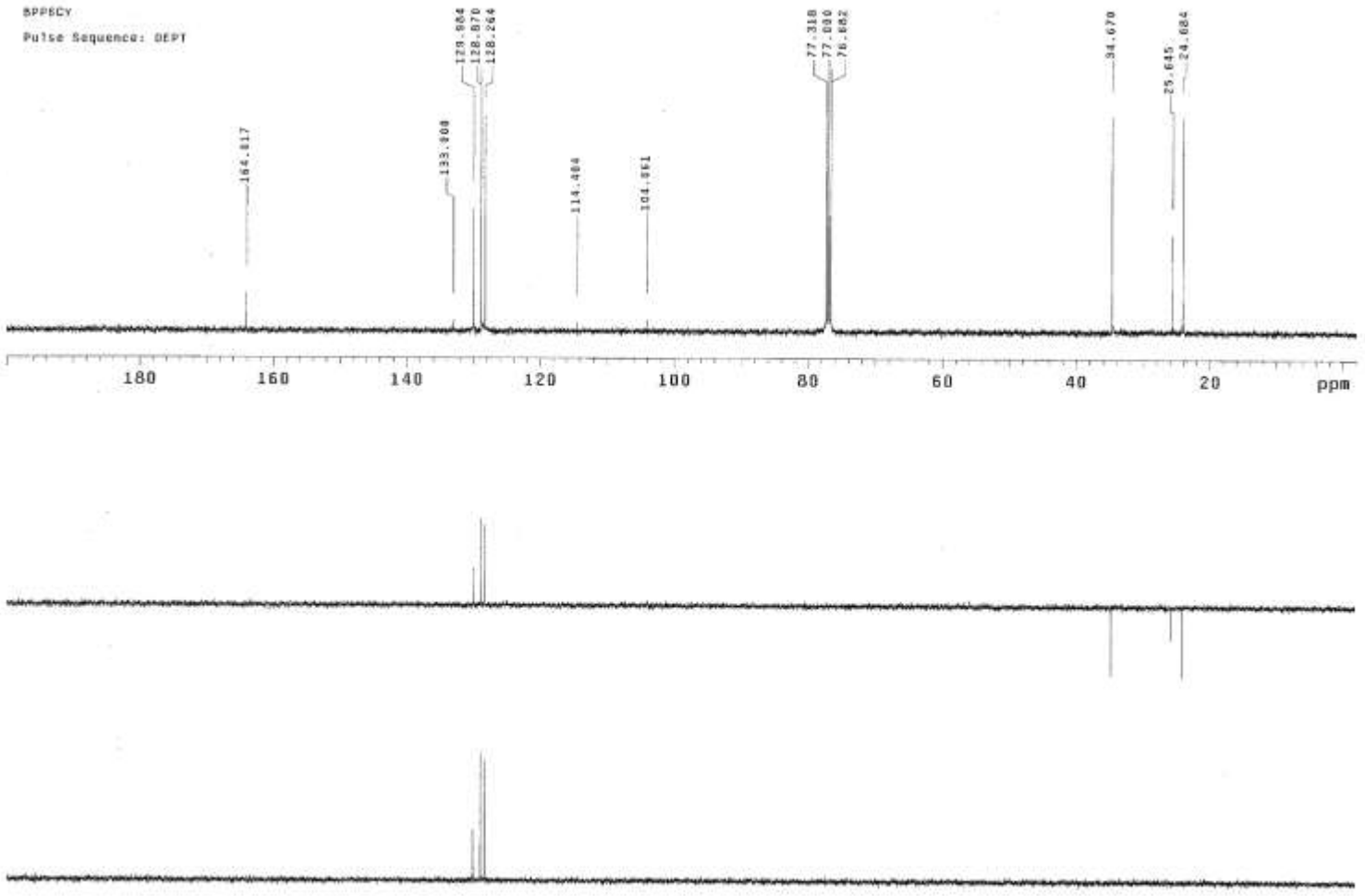


BPP6CY

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Dec 1 2014
Solvent: CDCl3
Ambient temperature
Total 8416 repetitions

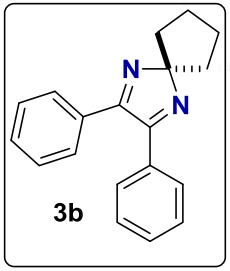


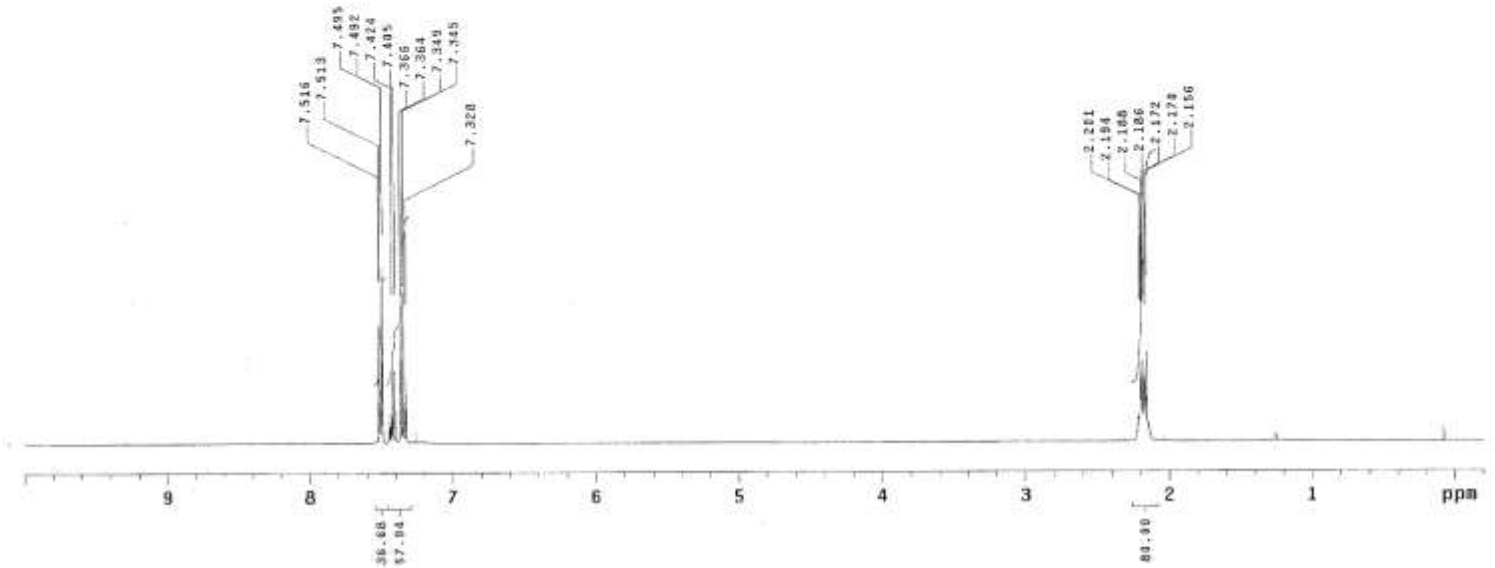

BPPSCY
Pulse Sequence: DEPT
164.817
133.808
129.864
128.870
128.264
114.484
104.961
77.318
77.000
76.682
34.670
25.645
24.684
180
160
140
120
100
80
60
40
20
ppm

BPPSCY

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Nov 20 2014
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

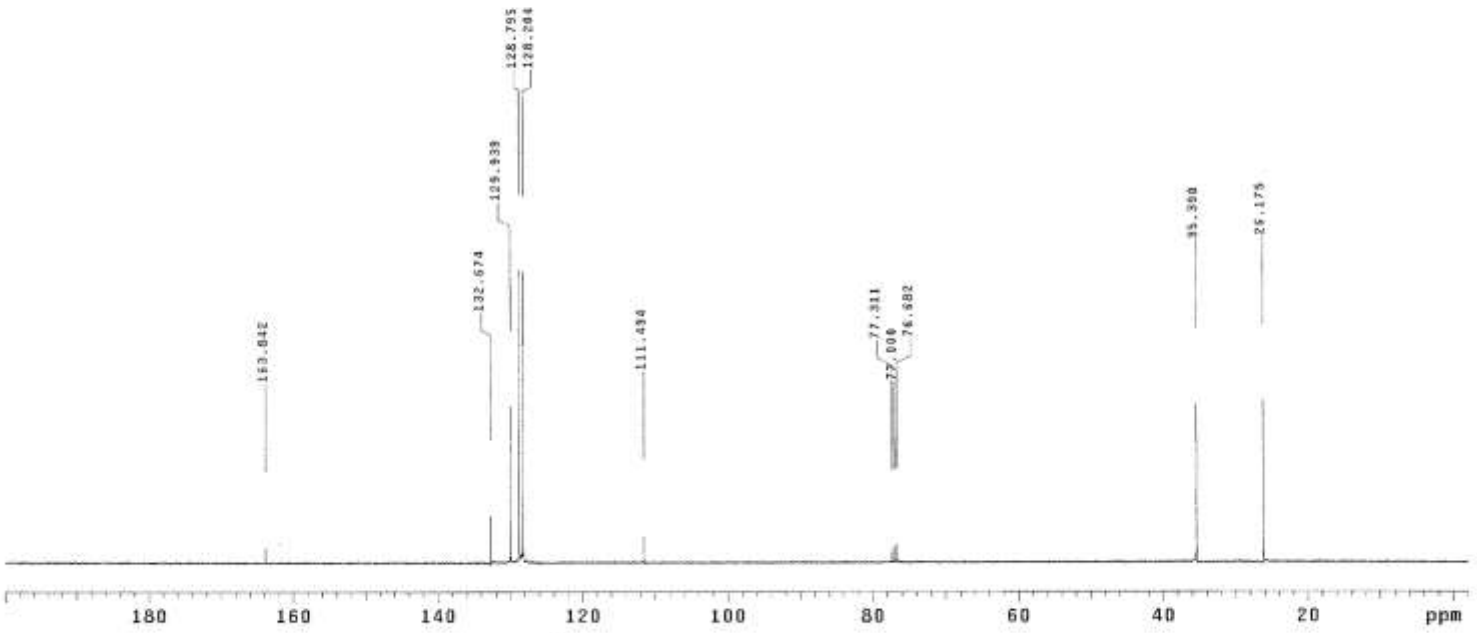


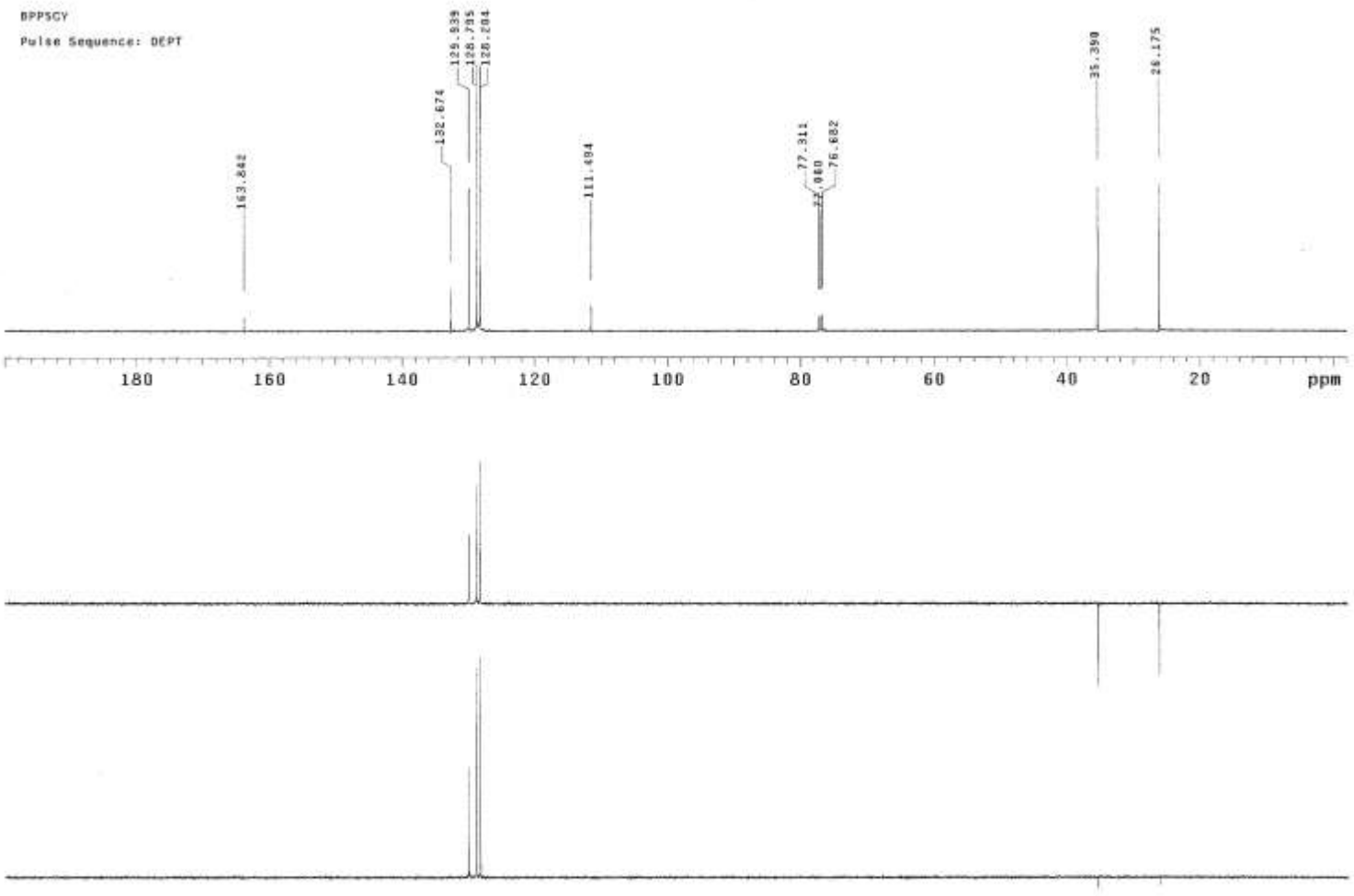


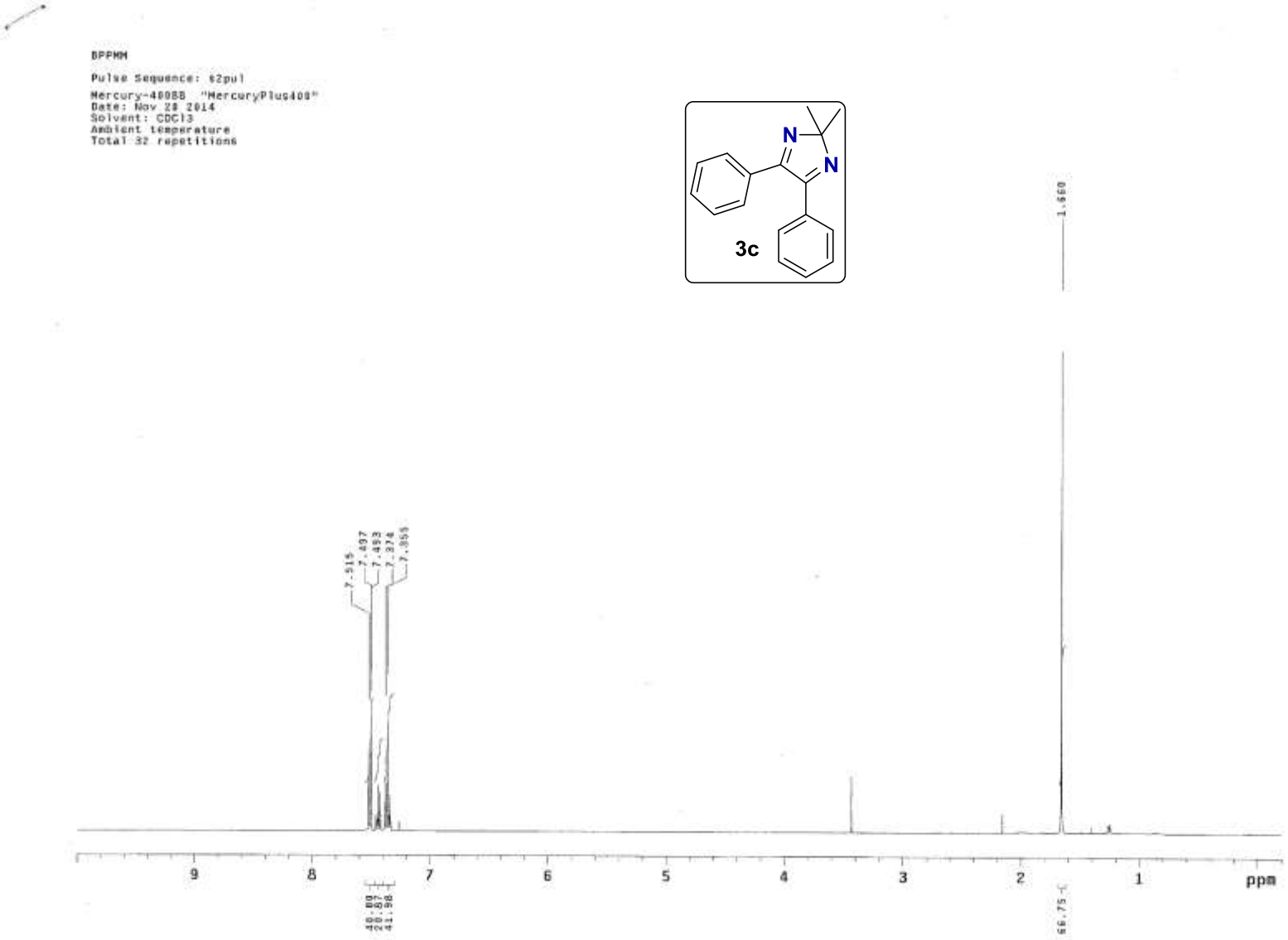
BPPSCY

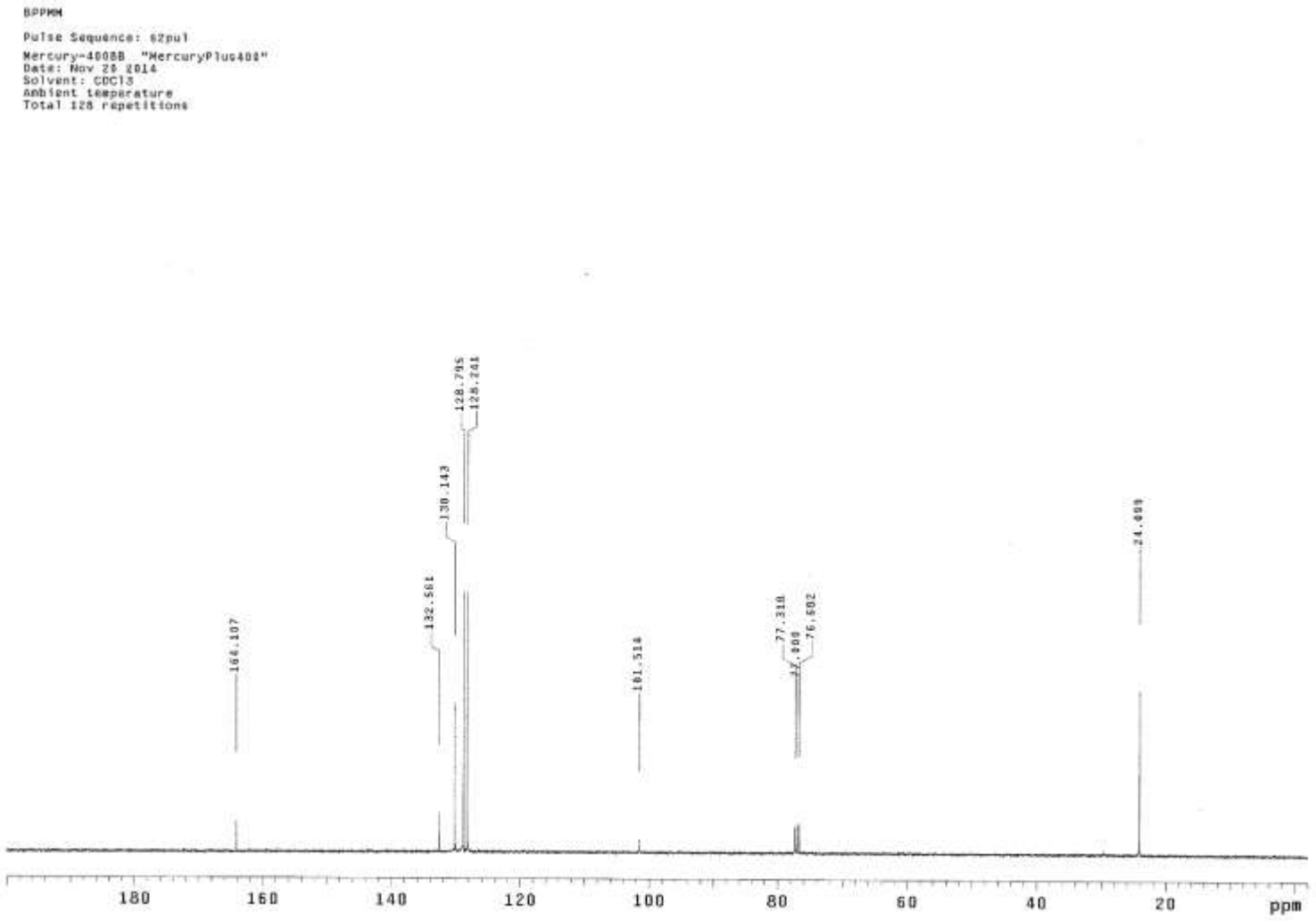
Pulse Sequence: s2pul

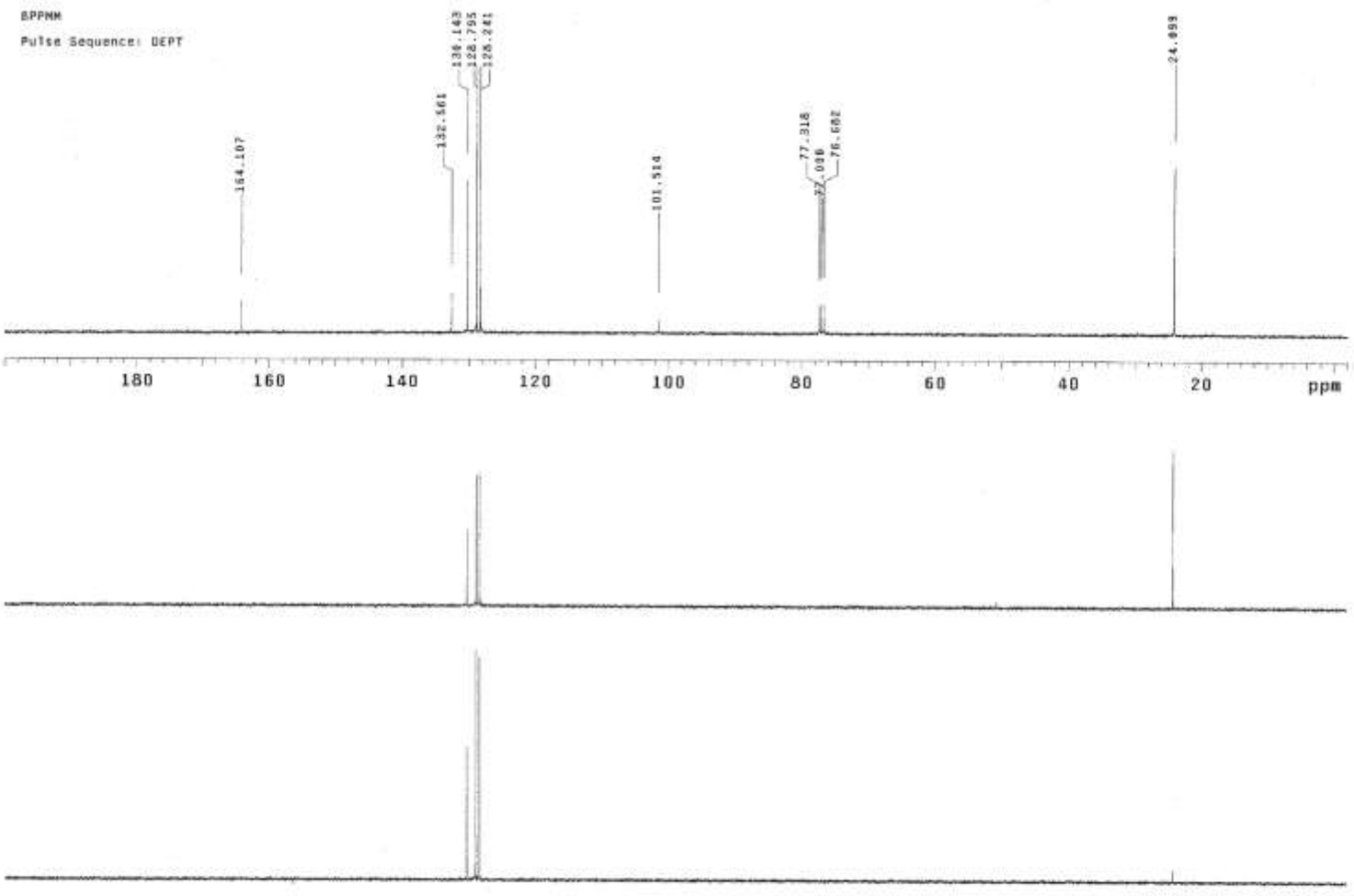
Mercury-400BB "MercuryPlus400"
Date: Nov 20 2014
Solvent: CDCl3
Ambient temperature
Total 168 repetitions




BPPSCY
Pulse Sequence: DEPT
163.842
132.674
129.939
128.735
128.284
111.494
77.311
77.060
76.682
35.390
26.175
180
160
140
120
100
80
60
40
20
ppm


BPPMM
Pulse Sequence: s2pul
Mercury-400BB "MercuryPlus400"
Date: Nov 28 2014
Solvent: CDCl3
Ambient temperature
Total 32 repetitions
3c
N
N
1.660
7.515
7.497
7.493
7.374
7.359
40.80
20.87
41.98
66.75
9
8
7
6
5
4
3
2
1
ppm

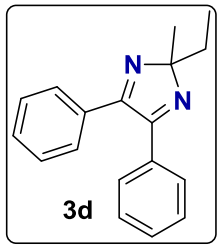

8PPHM
Pulse Sequence: 62pul
Mercury-400BB "MercuryPlus400"
Date: Nov 28 2014
Solvent: CDCl3
Ambient temperature
Total 128 repetitions
164.107
132.581
130.143
128.795
128.241
101.514
77.318
77.000
76.682
24.488
180
160
140
120
100
80
60
40
20
ppm

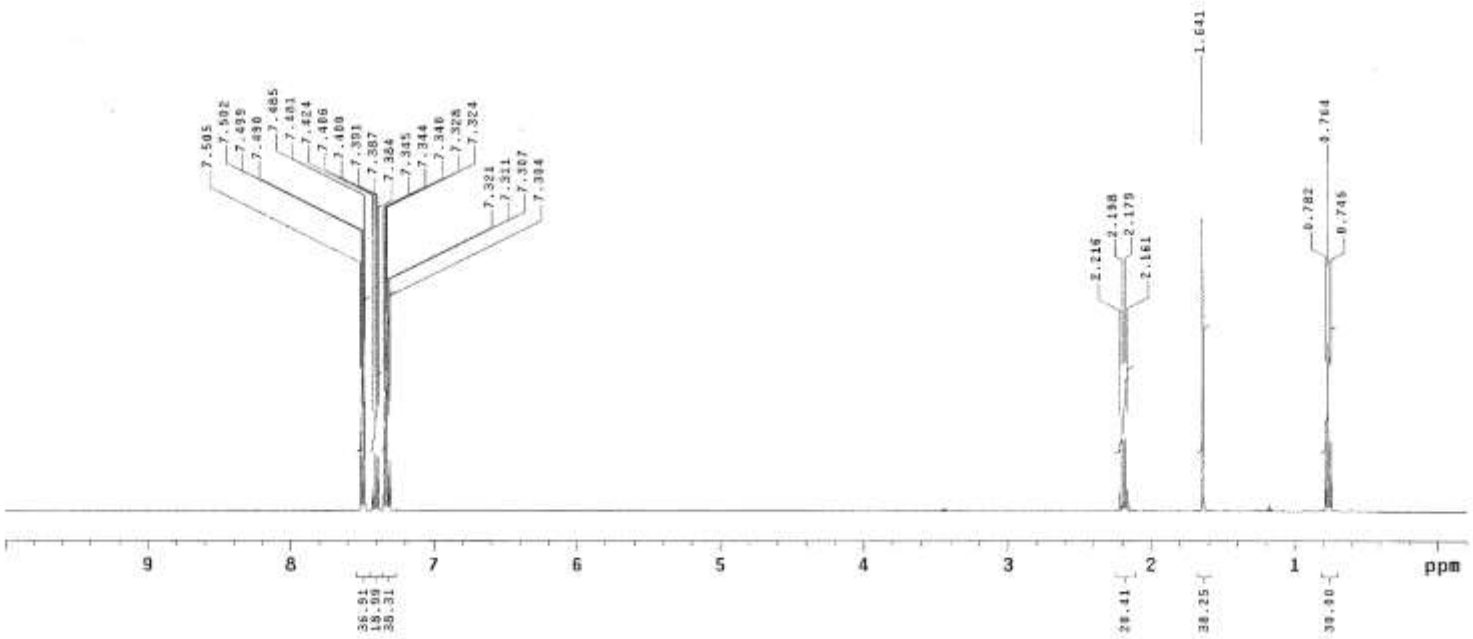

BPPNM
Pulse Sequence: DEPT
164.107
132.561
130.143
128.795
128.241
101.514
77.318
77.016
76.682
24.693
180
160
140
120
100
80
60
40
20
ppm

Hou-NB01-055

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Dec 11 2014
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

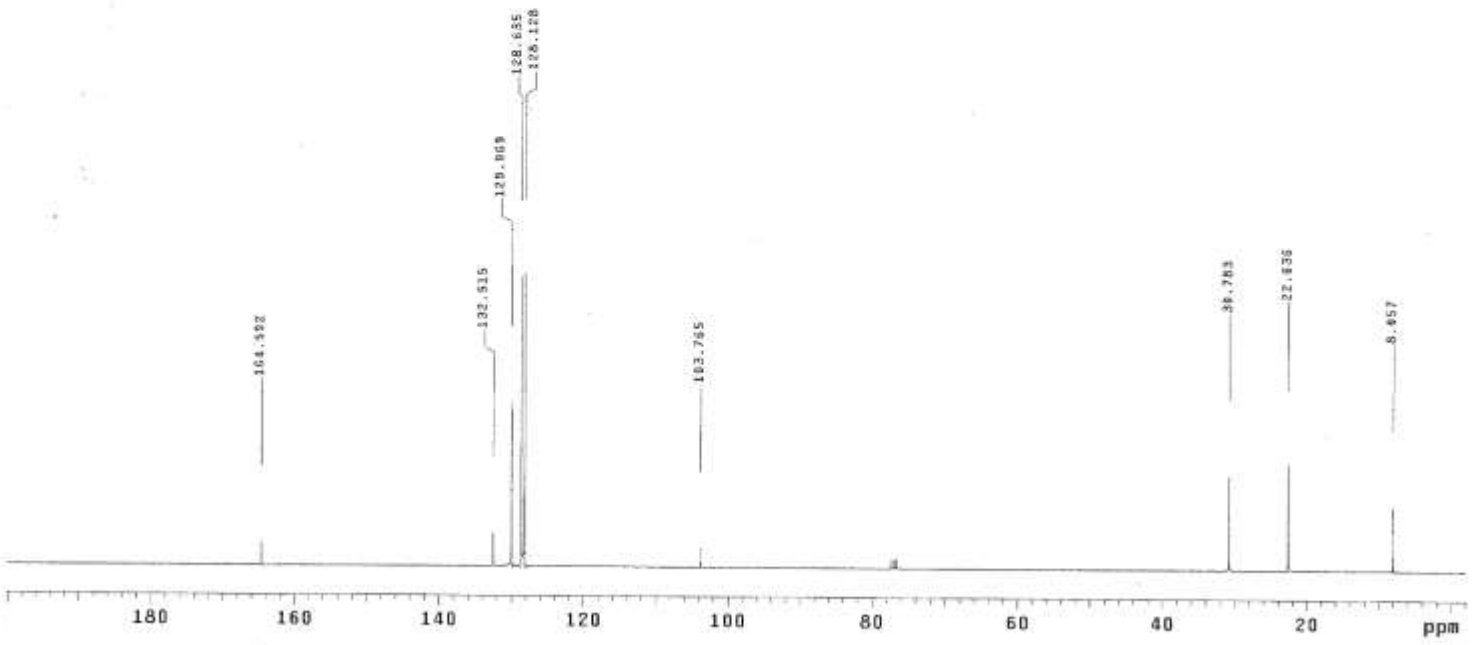


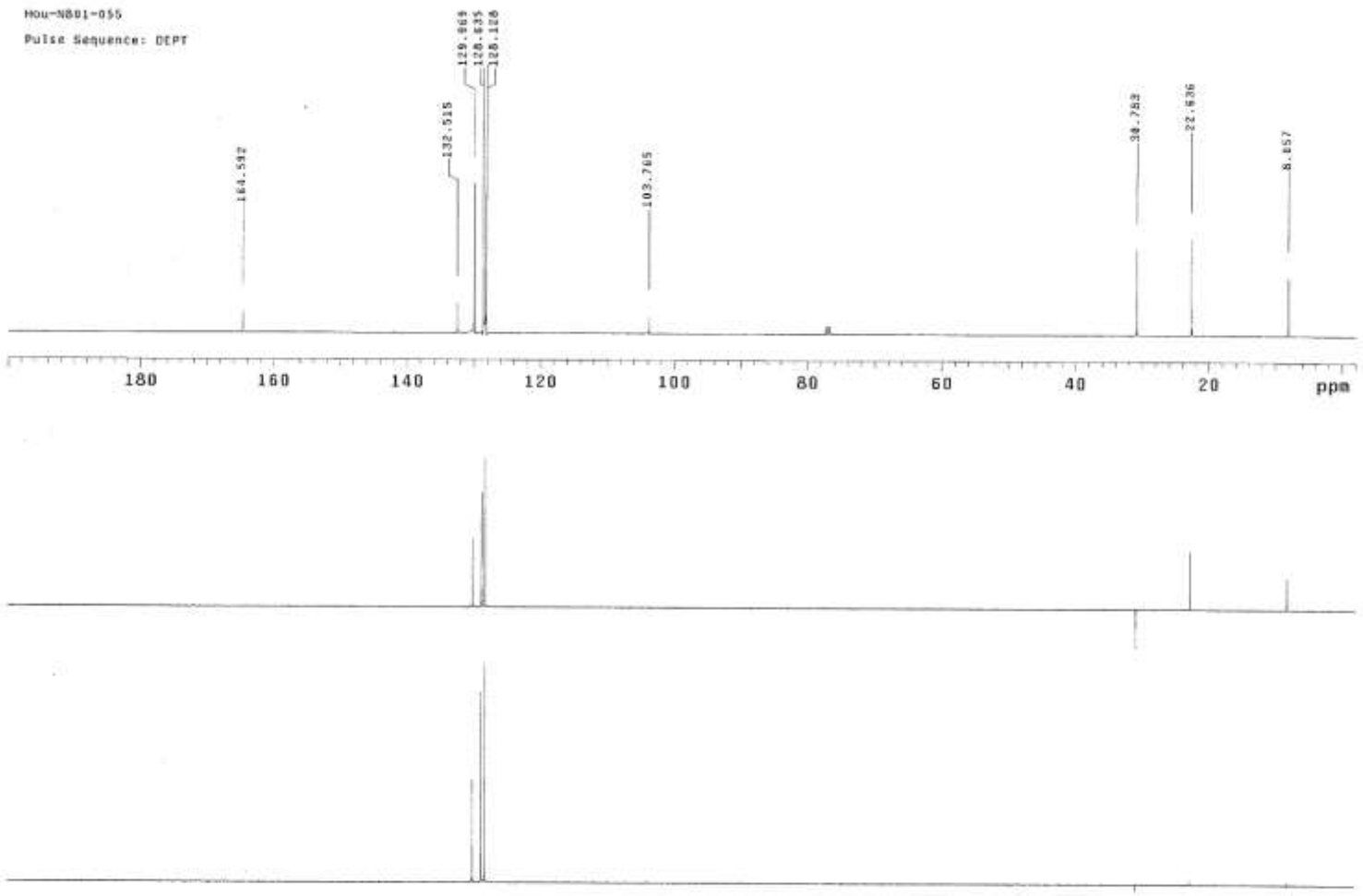


Hou-NB01-055

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Dec 11 2014
Solvent: CDCl3
Ambient temperature
Total 416 repetitions

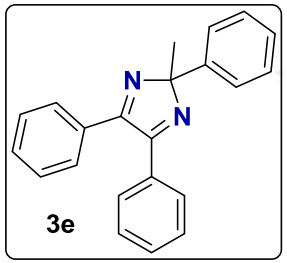



Hou-NB01-055
Pulse Sequence: DEPT
164.542
132.515
129.869
128.835
128.128
103.765
38.783
22.636
8.657
180
160
140
120
100
80
60
40
20
ppm

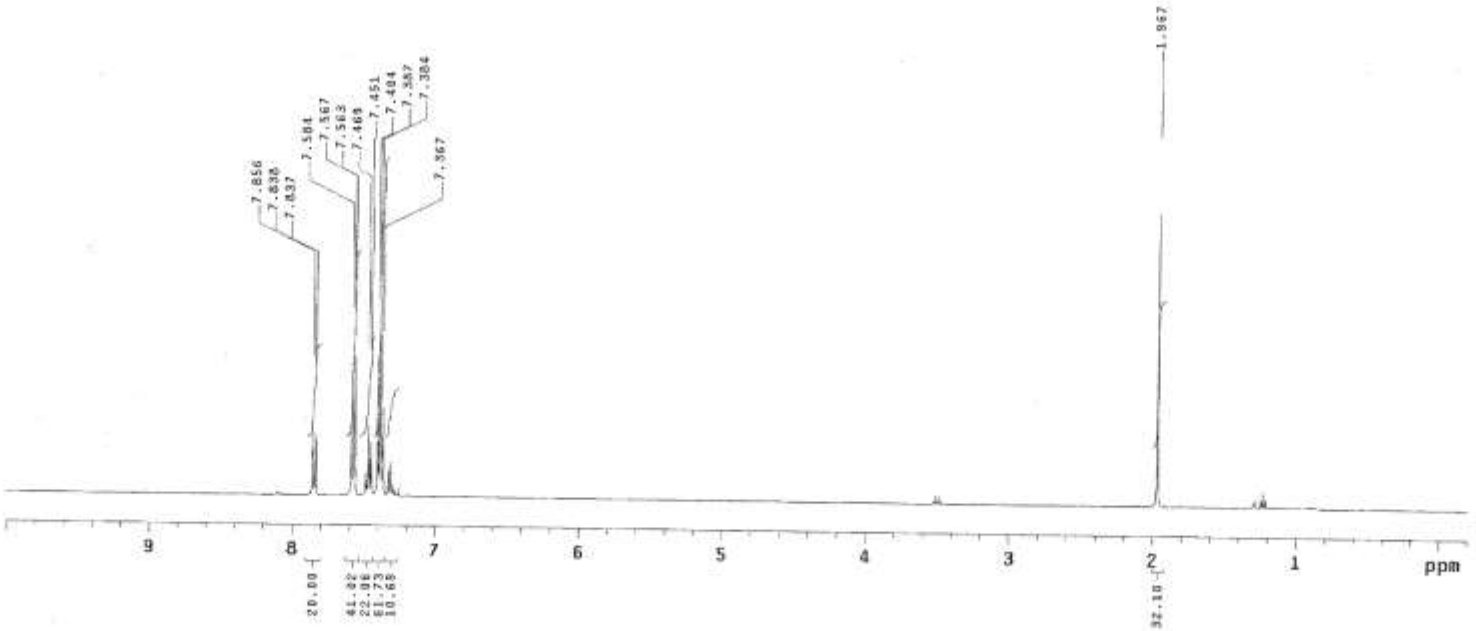
BPPMP

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Dec 1 2014
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



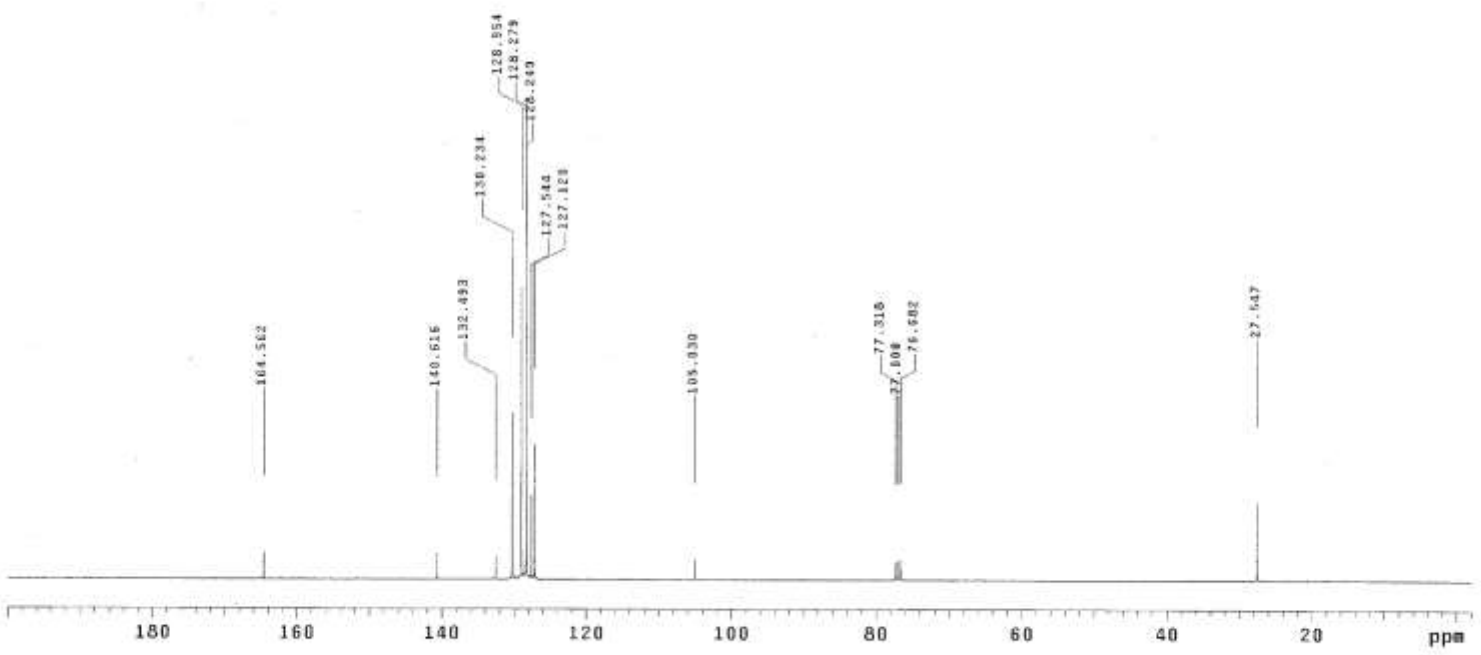
3e

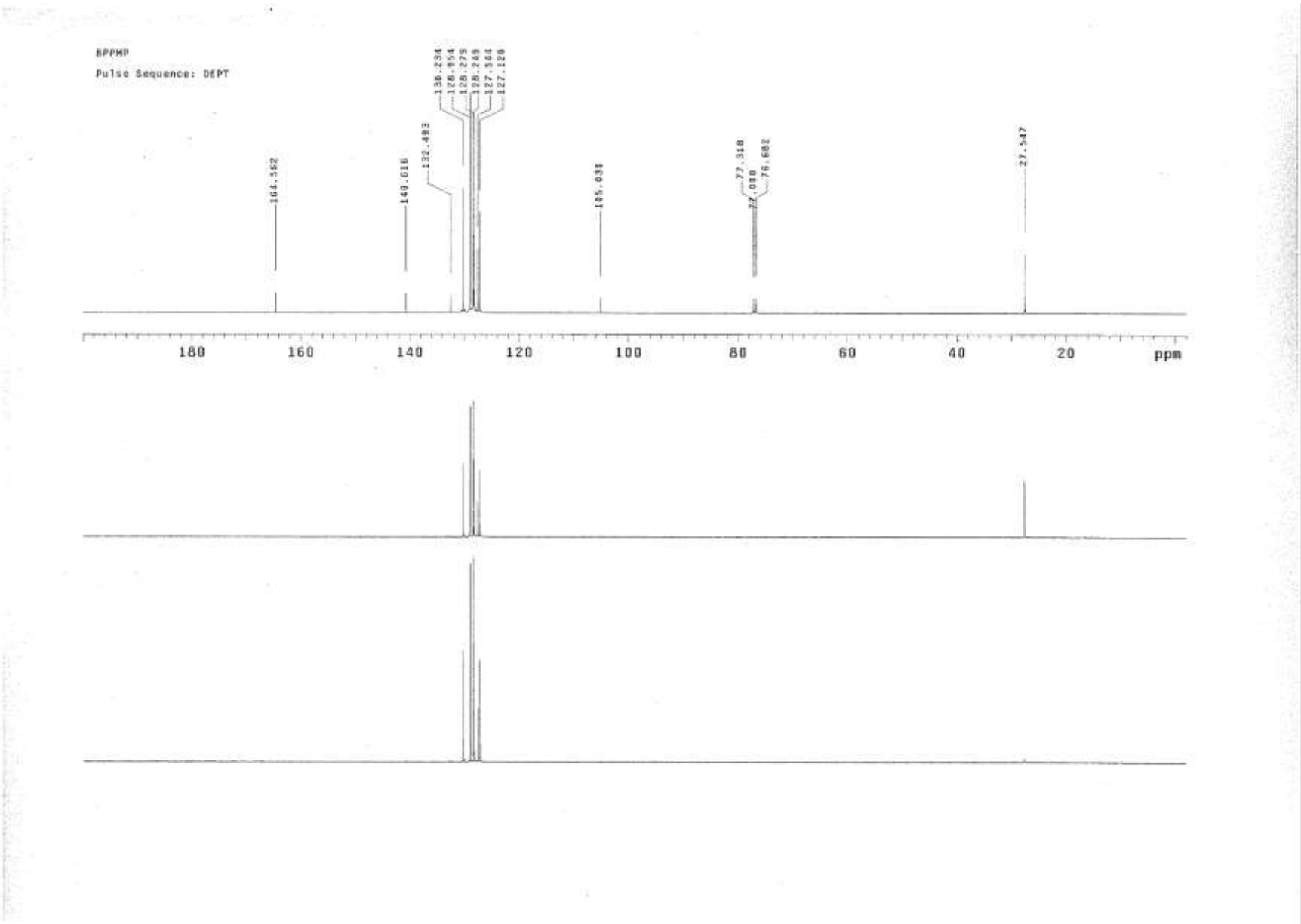


BPPMP

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Dec 1 2014
Solvent: CDCl3
Ambient temperature
Total 64000 repetitions

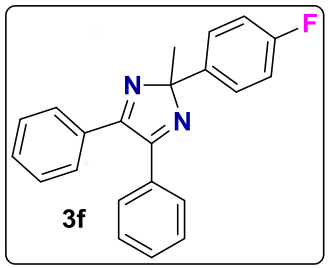


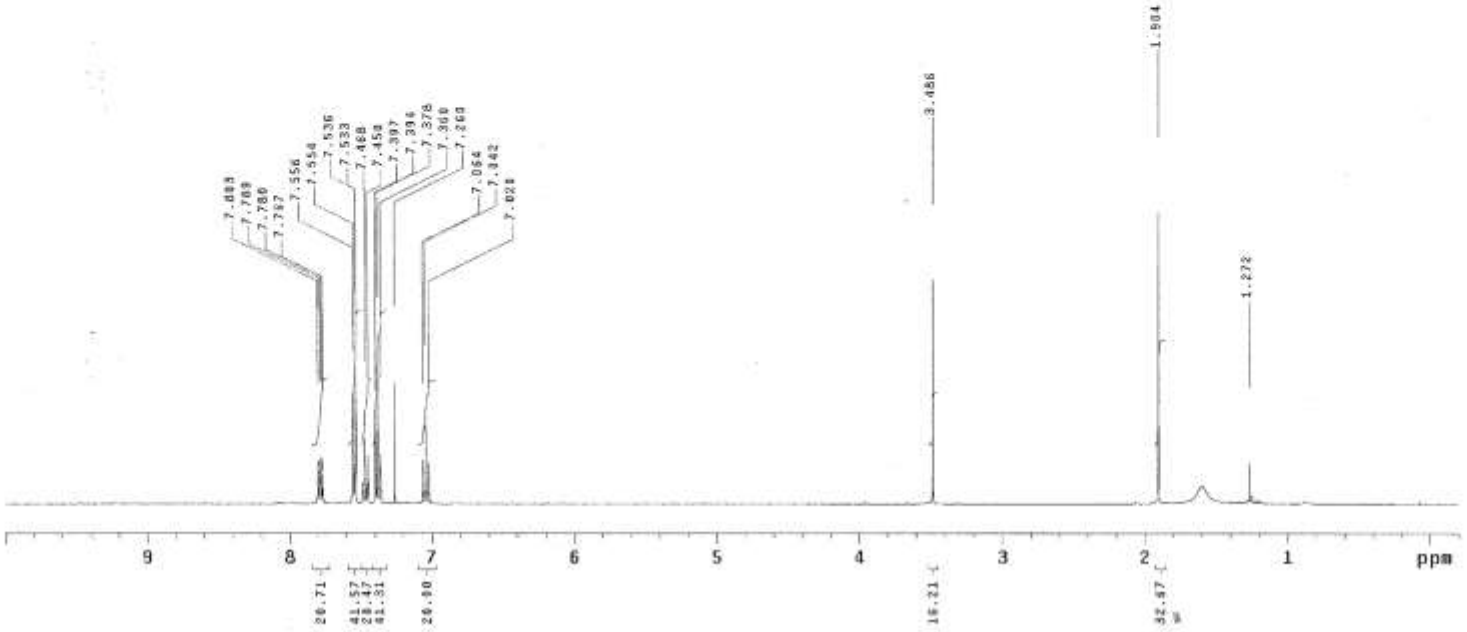

BPPMP
Pulse Sequence: DEPT
164.562
140.616
132.493
136.234
128.954
128.279
128.249
127.564
127.126
105.038
77.318
77.000
76.682
27.547
180
160
140
120
100
80
60
40
20
ppm

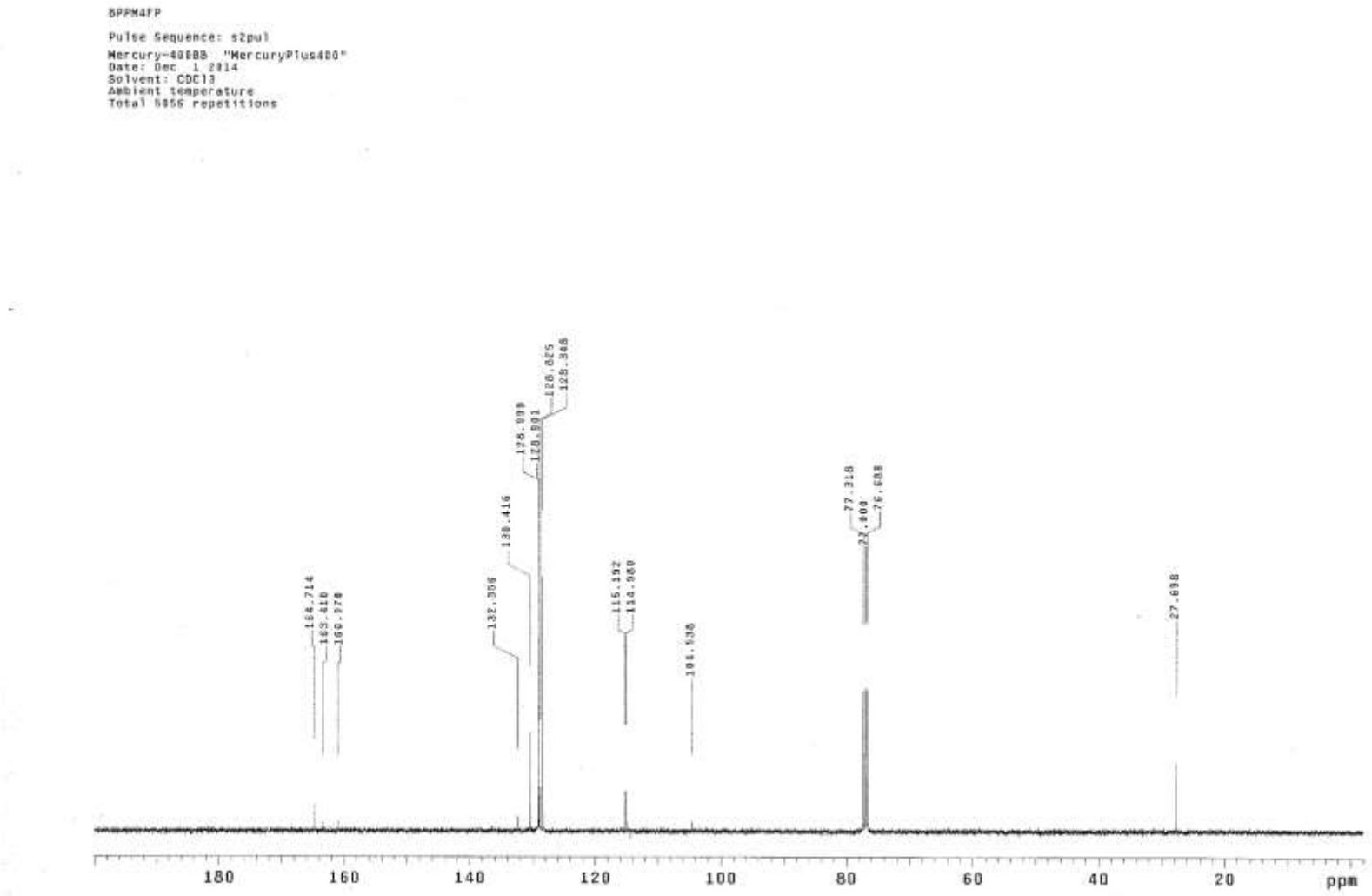
8PPM4FP

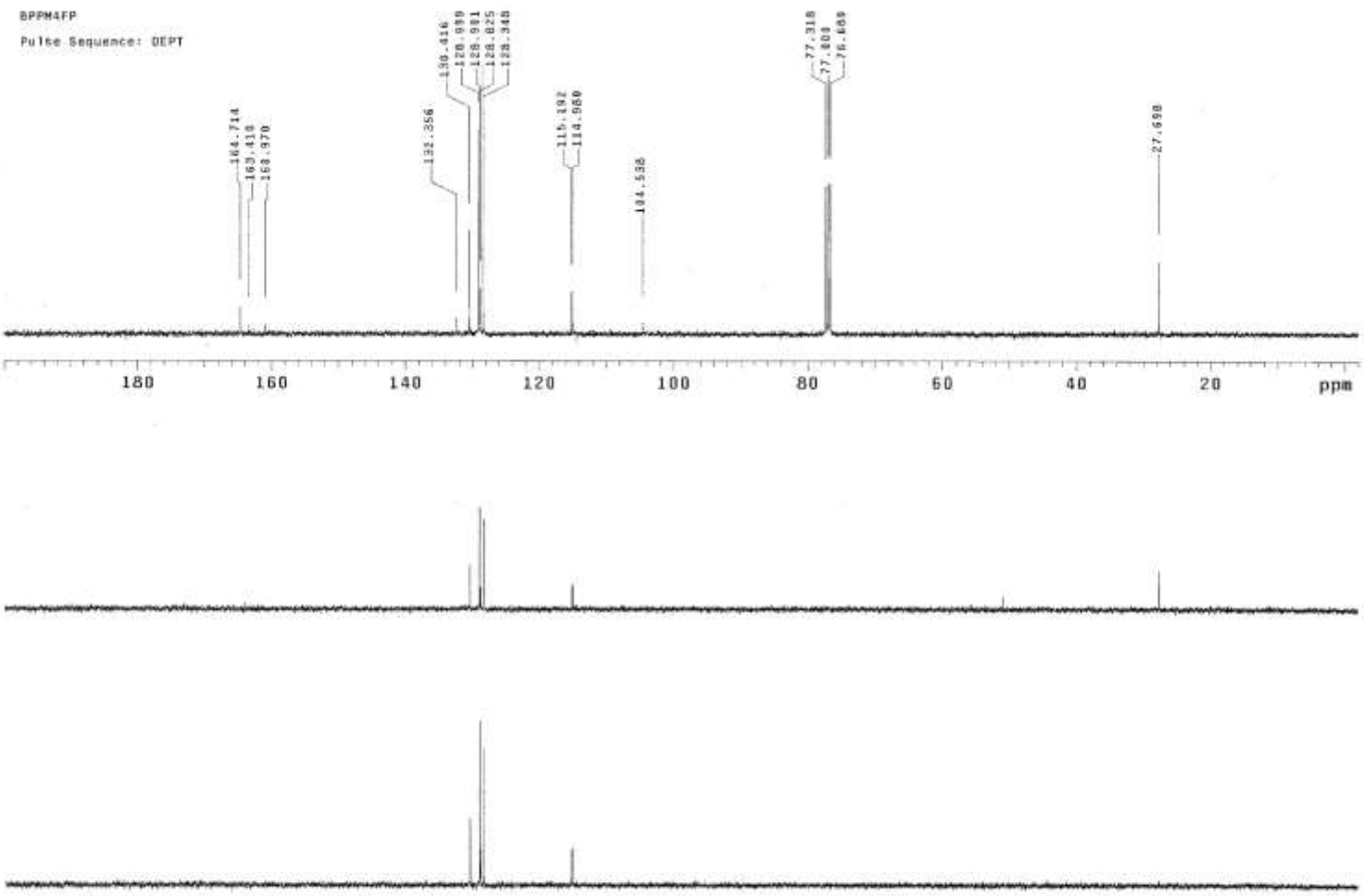
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Dec 1 2014
Solvent: CDCl3
Ambient temperature
Total 32 repetitions





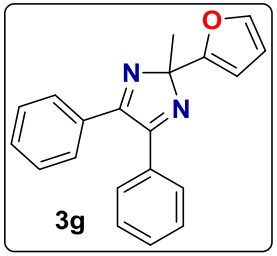

8PPM4FP
Pulse Sequence: s2pul
Mercury-400BB "MercuryPlus400"
Date: Dec 1 2014
Solvent: CDCl3
Ambient temperature
Total 5856 repetitions
164.714
163.410
160.978
132.356
130.416
128.939
128.891
128.825
128.348
115.192
114.980
104.536
77.318
77.000
76.688
27.698
180
160
140
120
100
80
60
40
20
ppm

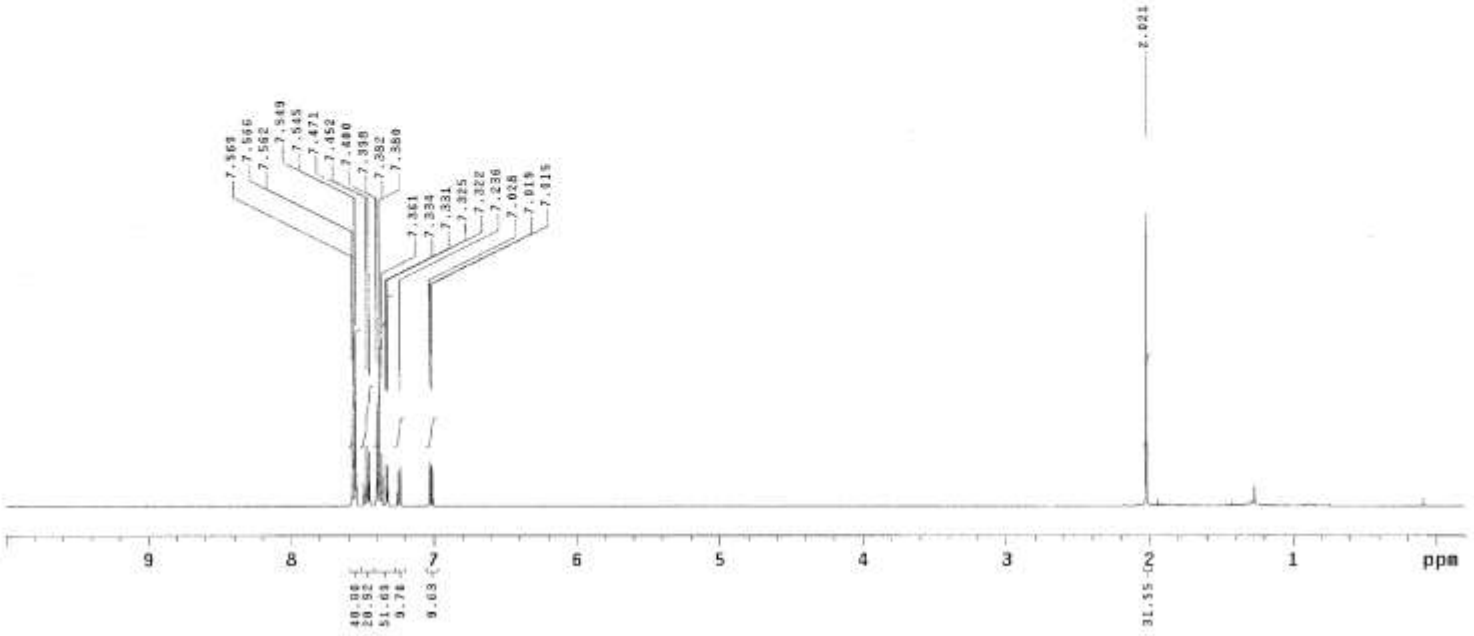

BPPM4FP
Pulse Sequence: DEPT
164.714
163.418
163.970
132.356
130.416
129.959
129.981
128.825
128.348
115.192
114.960
104.538
77.318
77.000
76.680
27.698
180
160
140
120
100
80
60
40
20
ppm

8PPMOSCV

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Nov 19 2014
Solvent: CDCl3
Ambient temperature
File: M0282-7
Total 32 repetitions

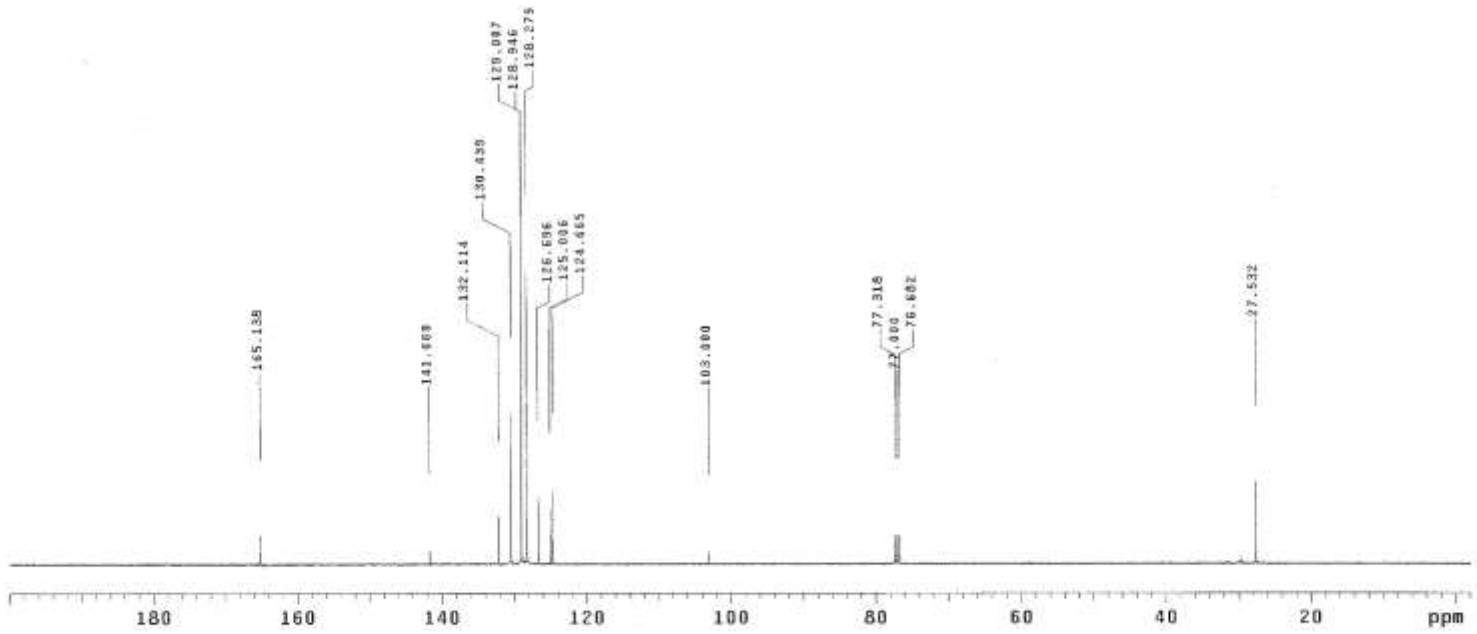


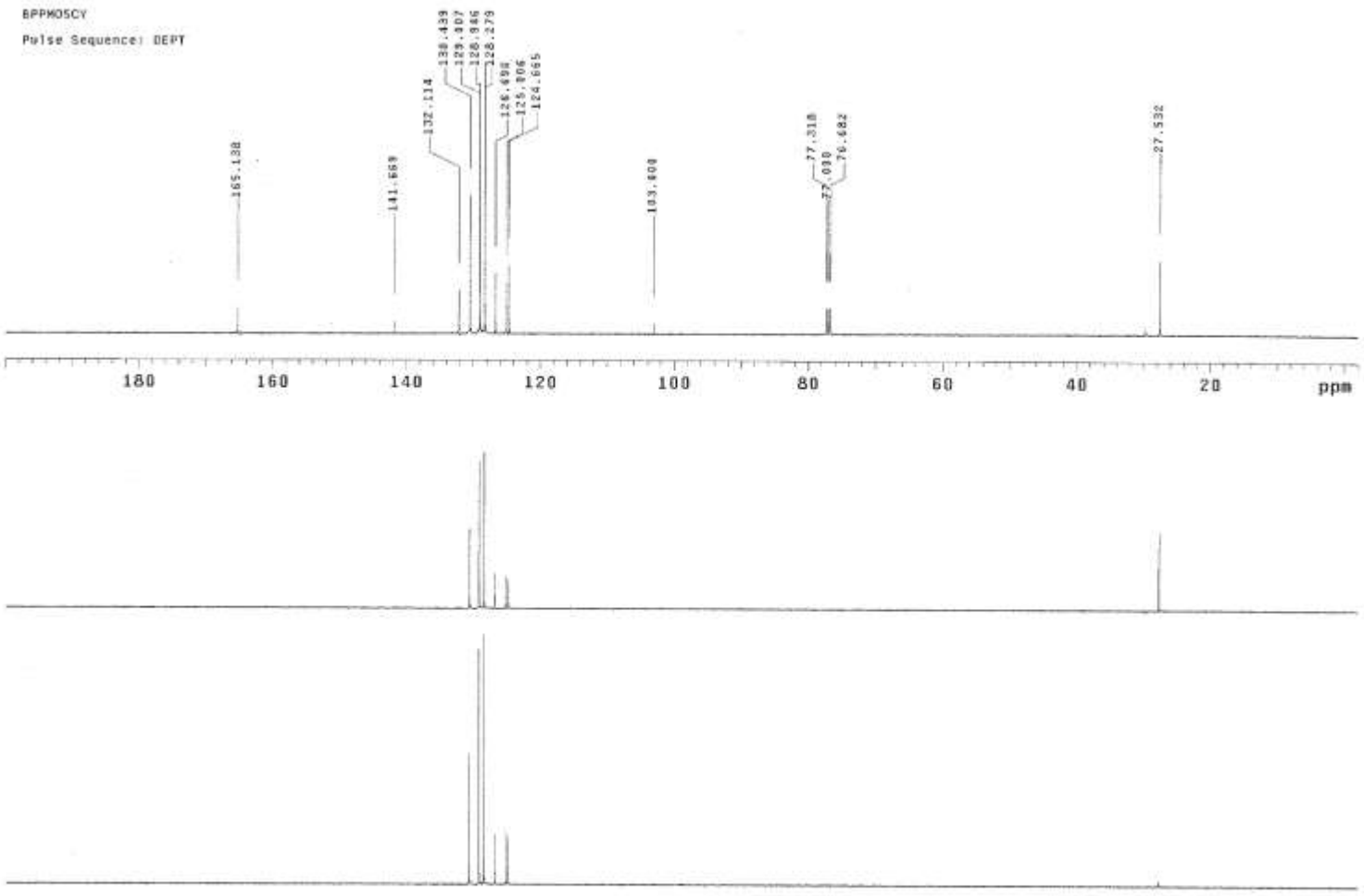


8PFMD5CY

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Nov 19 2014
Solvent: CDCl3
Ambient temperature
File: MB282-8
Total 418 repetitions

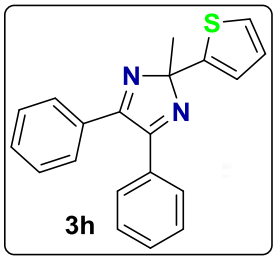


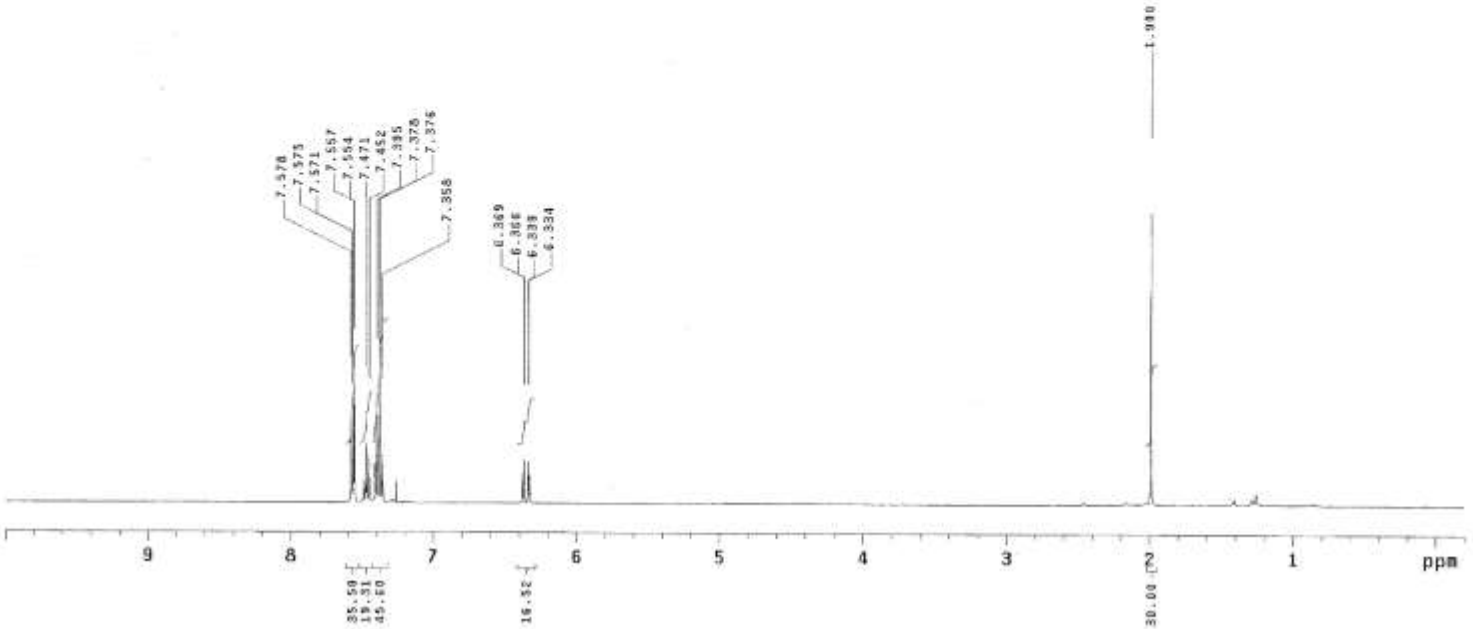

BPPMOSCY
Pulse Sequence: DEPT
165.138
141.669
132.114
130.439
129.307
128.946
128.279
126.698
125.806
124.665
103.600
77.318
77.000
76.682
27.532
180
160
140
120
100
80
60
40
20
ppm

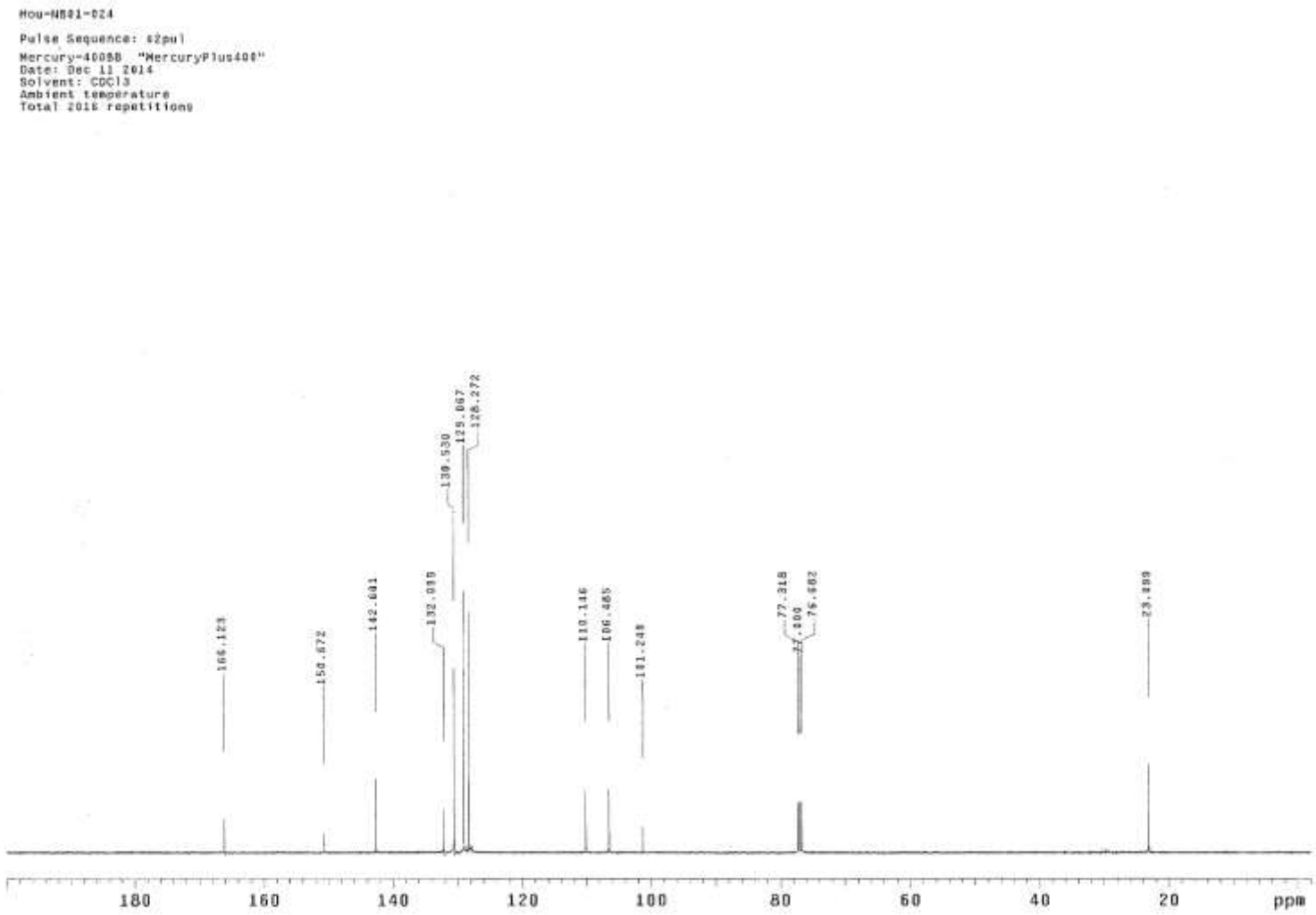
Hou-NB01-024

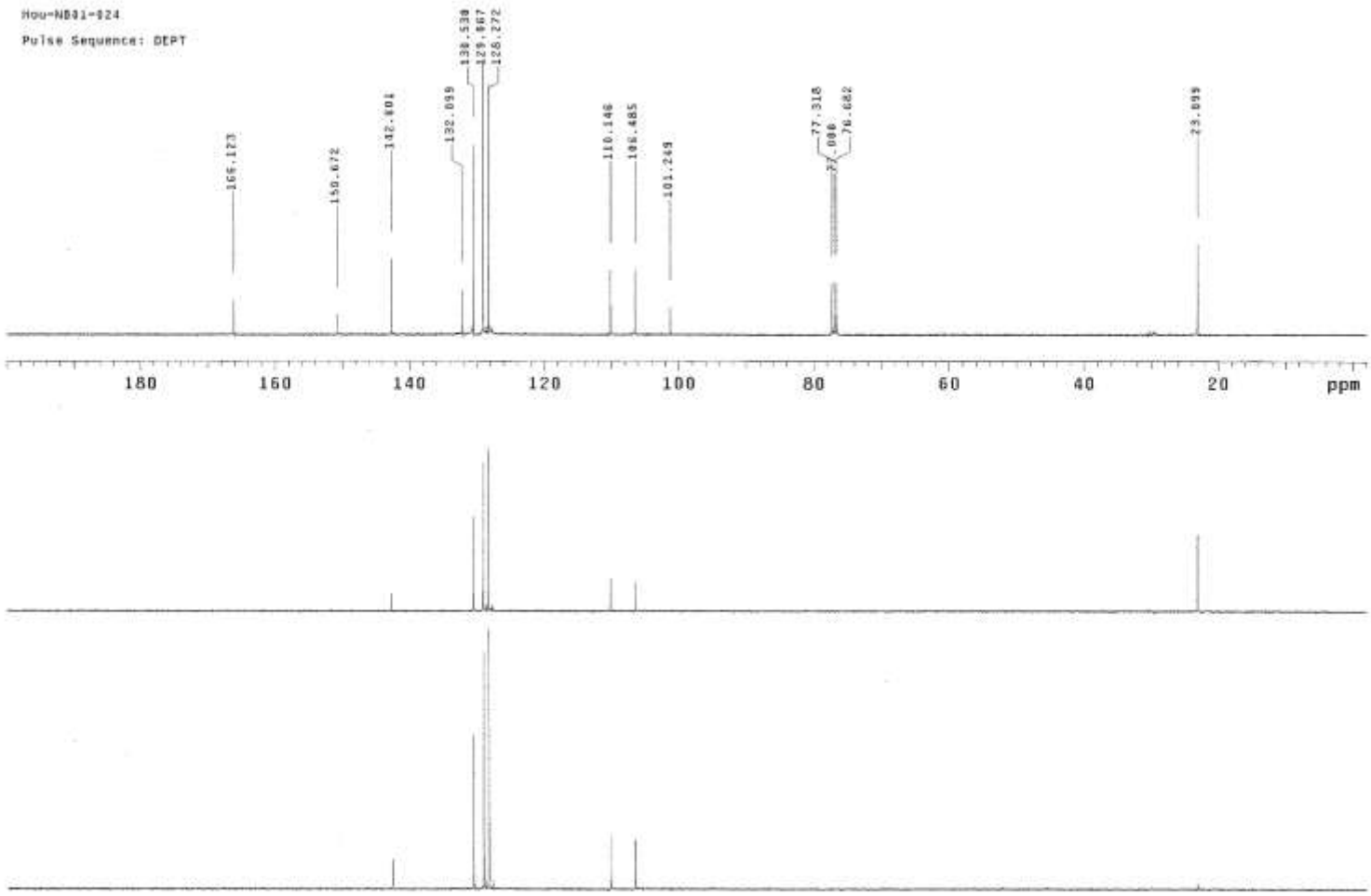
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Dec 11 2014
Solvent: CDCl3
Ambient temperature
Total 32 repetitions





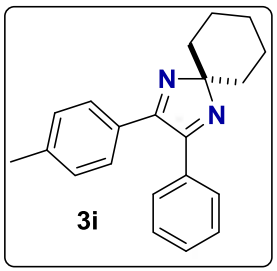

Hou-NB01-024
Pulse Sequence: s2pul
Mercury-400BB "MercuryPlus400"
Date: Dec 11 2014
Solvent: CDCl3
Ambient temperature
Total 2016 repetitions
166.123
150.672
142.041
132.035
130.530
129.067
128.272
118.146
106.465
101.248
77.318
77.000
76.682
23.899
180
160
140
120
100
80
60
40
20
ppm


Hou-NB01-024
Pulse Sequence: DEPT
166.123
150.672
142.801
132.059
130.530
129.867
128.272
110.146
108.485
101.249
77.318
77.000
76.682
23.099
180
160
140
120
100
80
60
40
20
ppm

B4PP6CY

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Nov 20 2014
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



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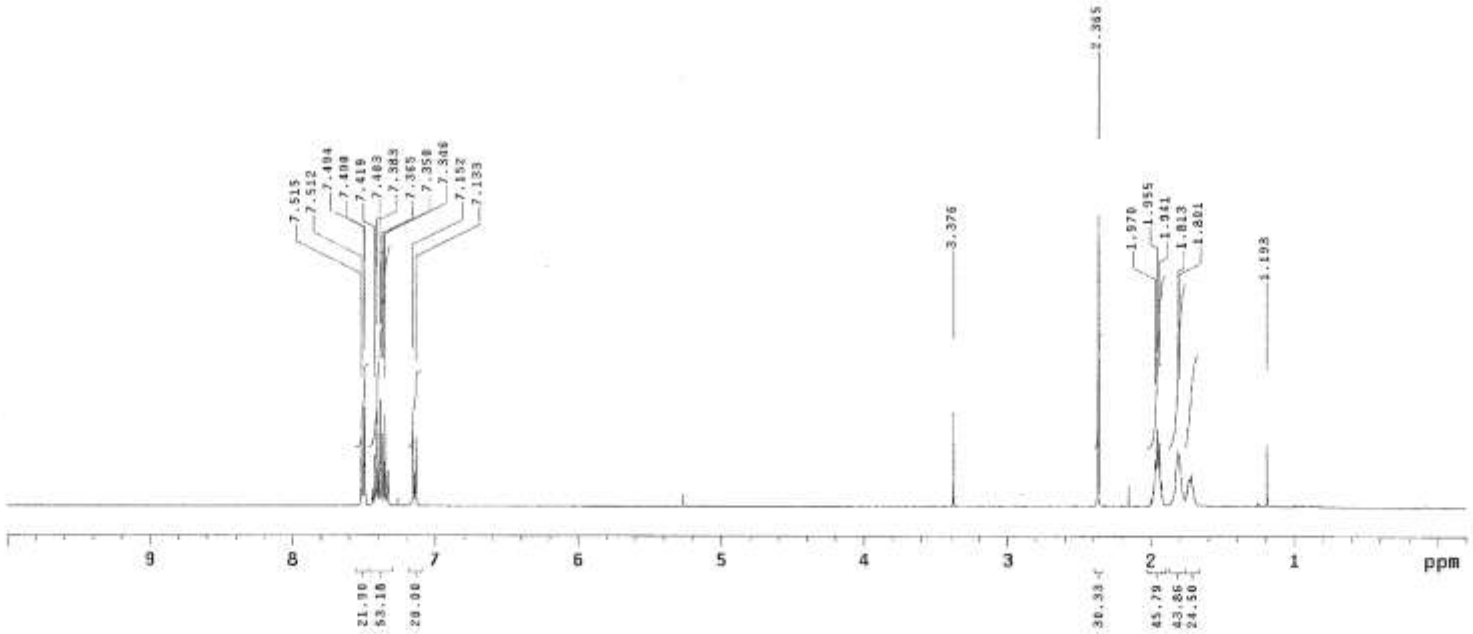
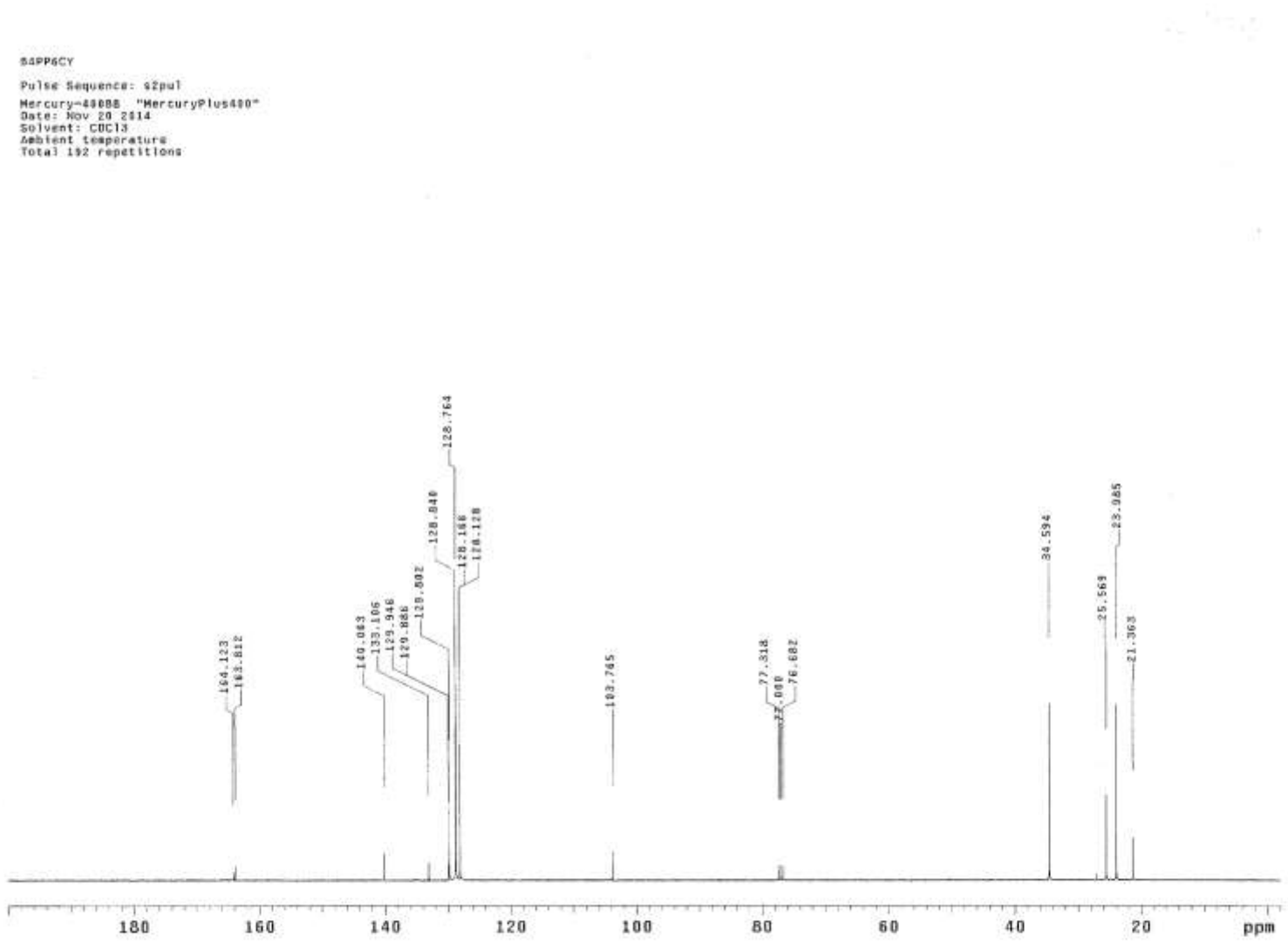
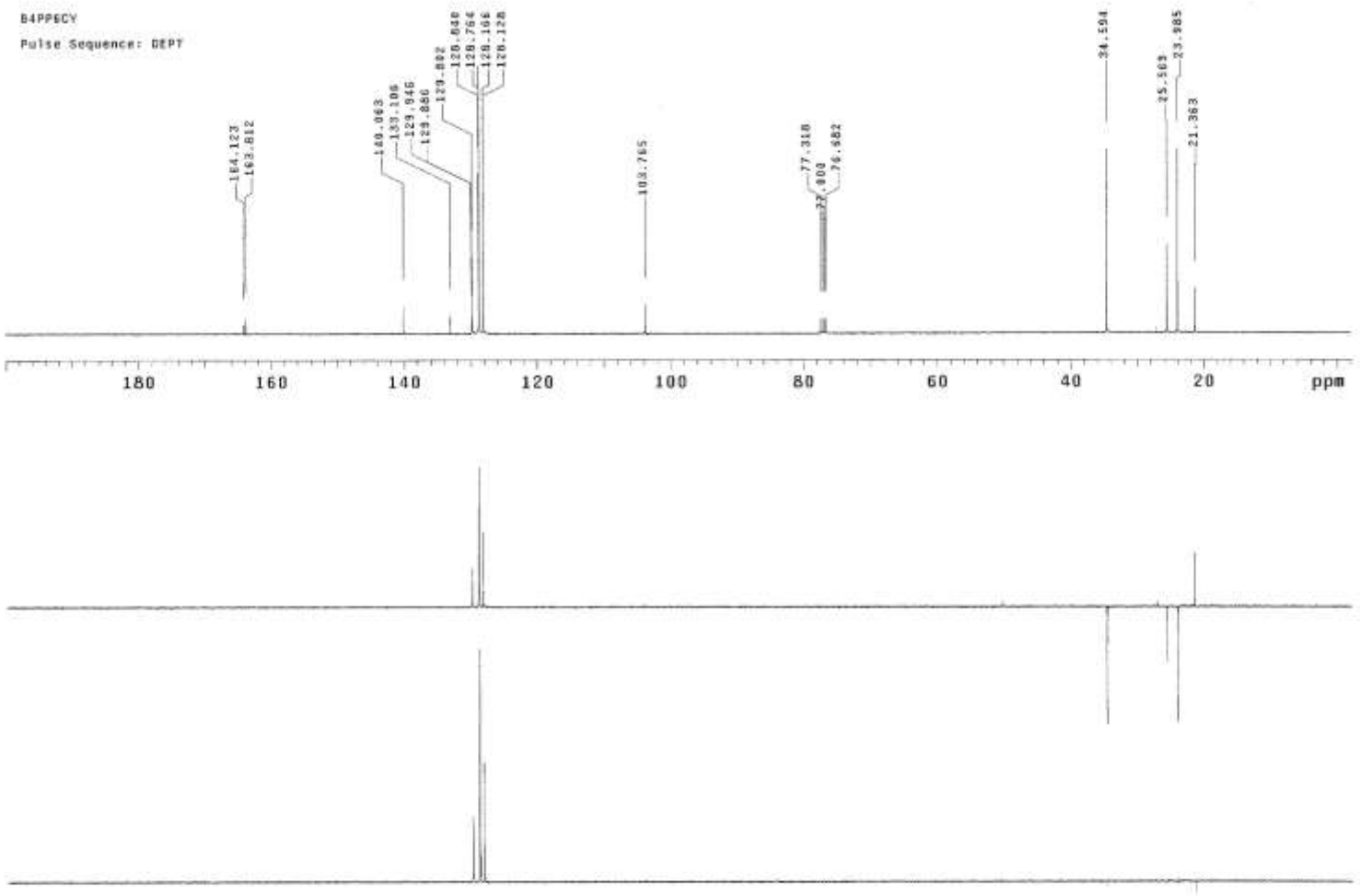


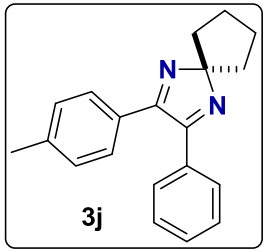

S4PP6CY
Pulse Sequence: s2pul
Mercury-400BB "MercuryPlus400"
Date: Nov 20 2014
Solvent: CDCl3
Ambient temperature
Total 192 repetitions
164.123
163.812
140.063
133.106
129.946
129.886
129.682
128.848
128.764
128.148
128.128
103.745
77.318
77.000
76.682
34.594
25.563
23.985
21.363
180
160
140
120
100
80
60
40
20
ppm


B4PP6CY
Pulse Sequence: DEPT
164.123
163.812
140.063
133.106
129.946
129.886
129.882
128.648
128.764
128.166
126.128
103.765
77.318
77.000
76.682
34.594
25.563
23.985
21.363
180
160
140
120
100
80
60
40
20
ppm

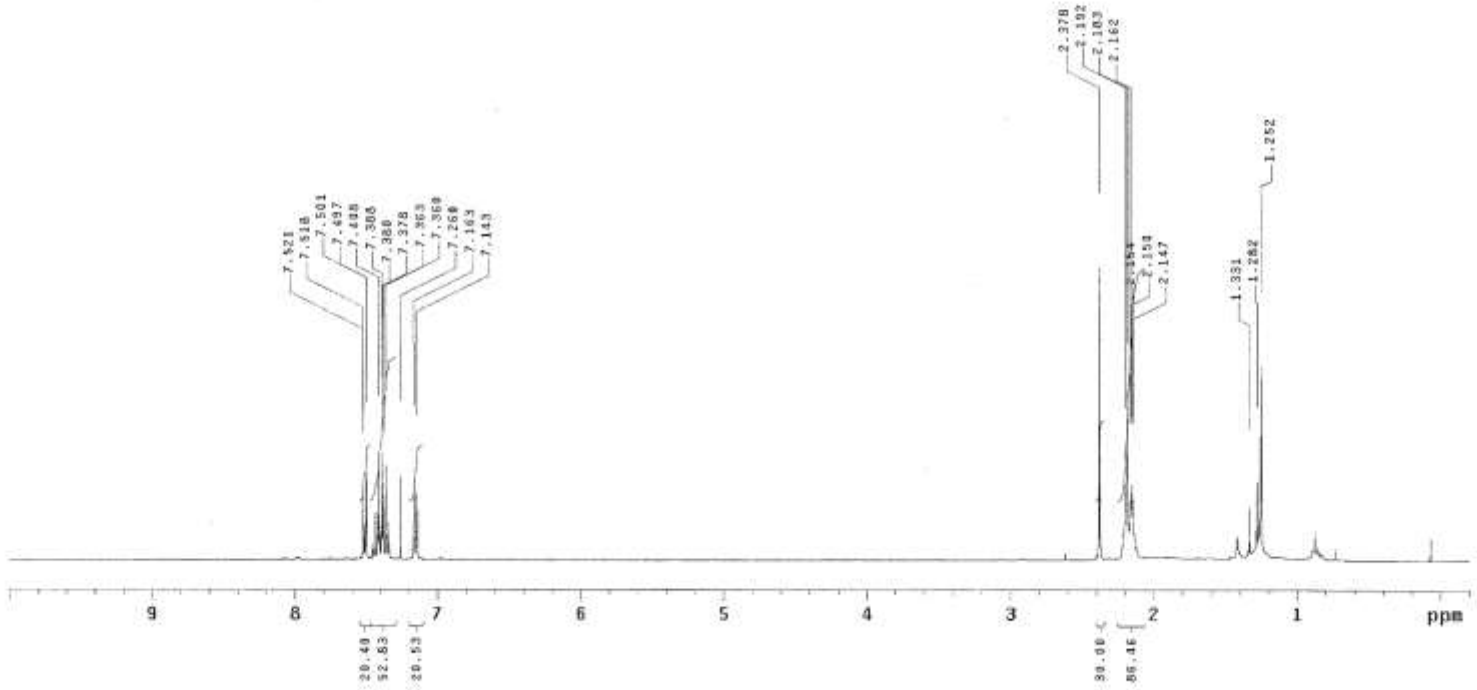
84MPPSCY

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Nov 19 2014
Solvent: CDCl3
Ambient temperature
File: M0282-10
Total 32 repetitions



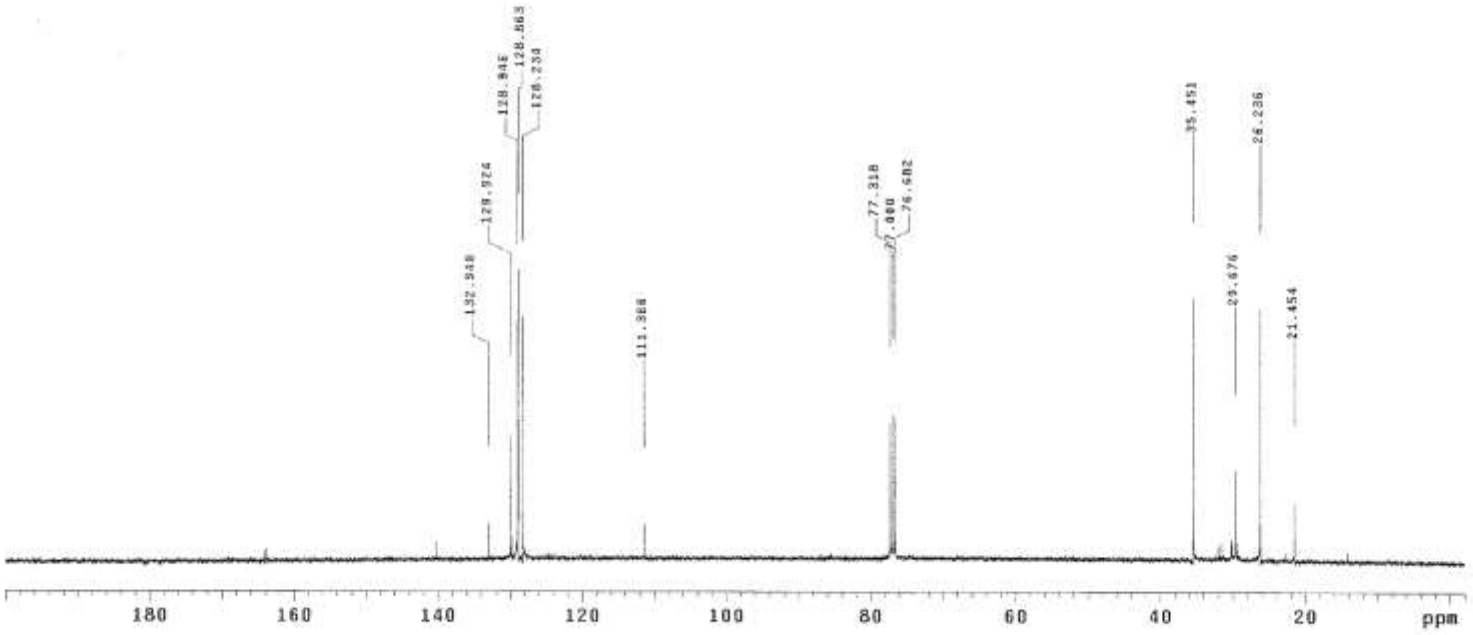
3j

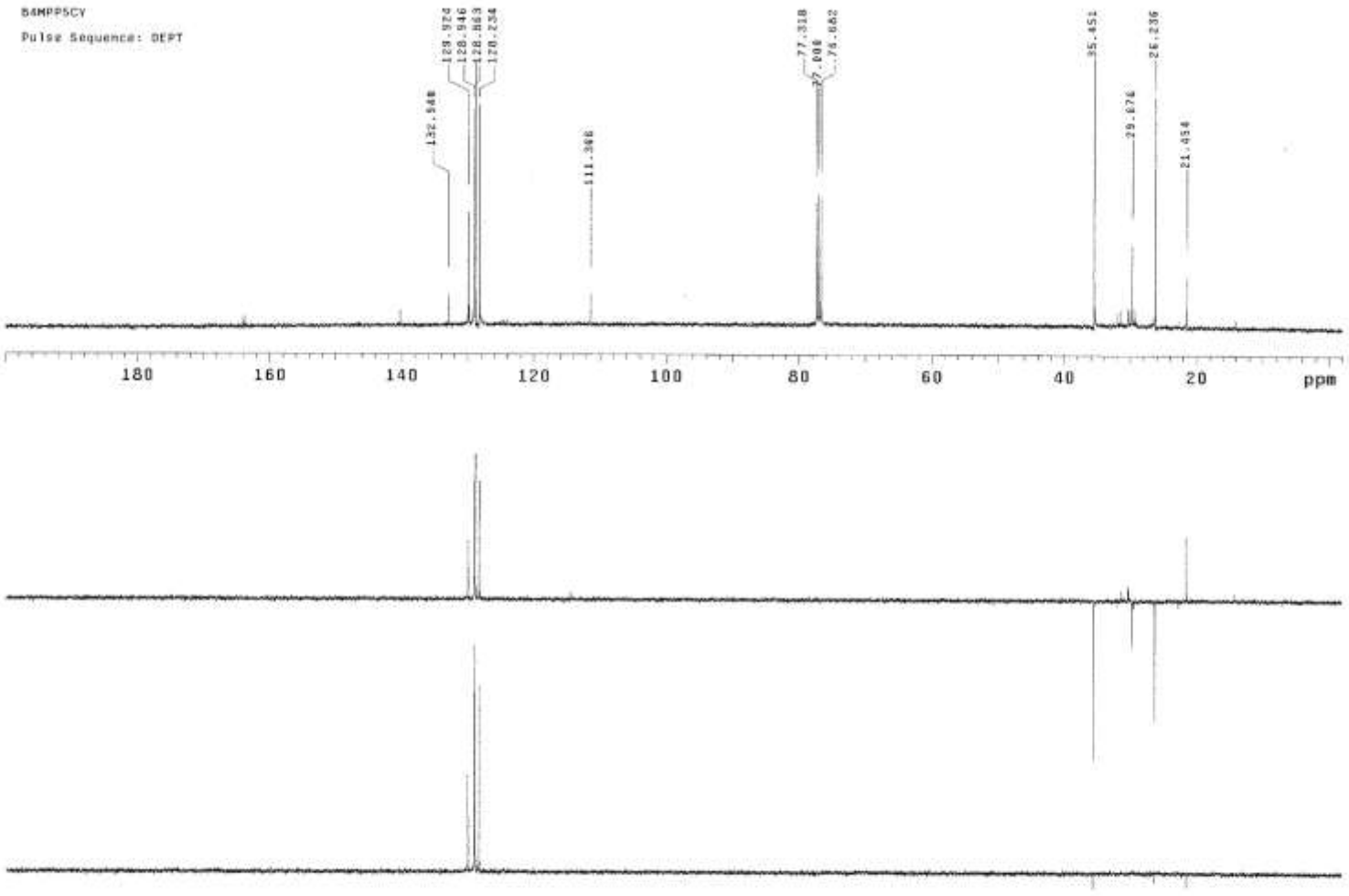


B4MPPSCY

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Nov 13 2014
Solvent: CDCl3
Ambient temperature
File: M0282-11
Total 4608 repetitions

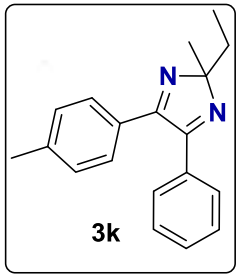


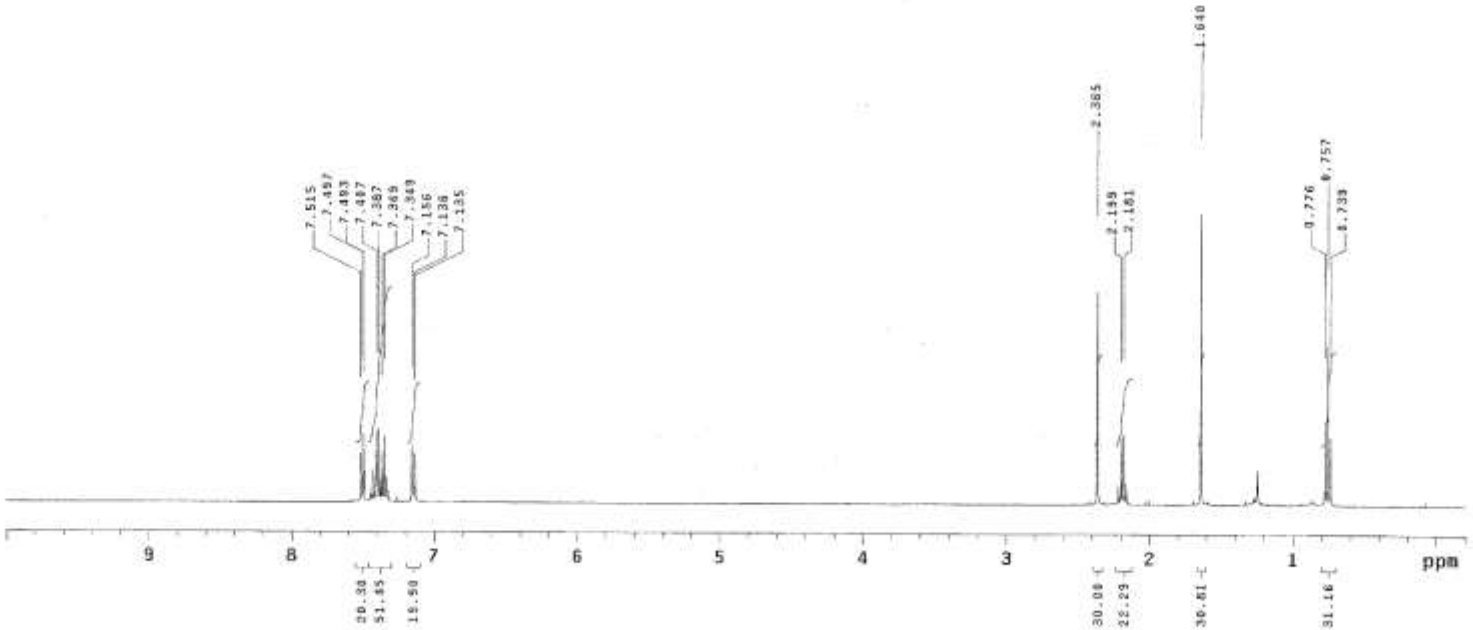

B4MPP5CY
Pulse Sequence: DEPT
132.548
129.924
128.946
128.863
120.234
111.366
77.318
77.000
76.682
35.451
29.076
26.236
21.454
180
160
140
120
100
80
60
40
20
ppm

B4MPPME

Pulse Sequence: s2pul

Mercury=400BB "MercuryPlus400"
Date: Nov 19 2014
Solvent: CDCl3
Ambient temperature
File: M0282-13
Total 64 repetitions

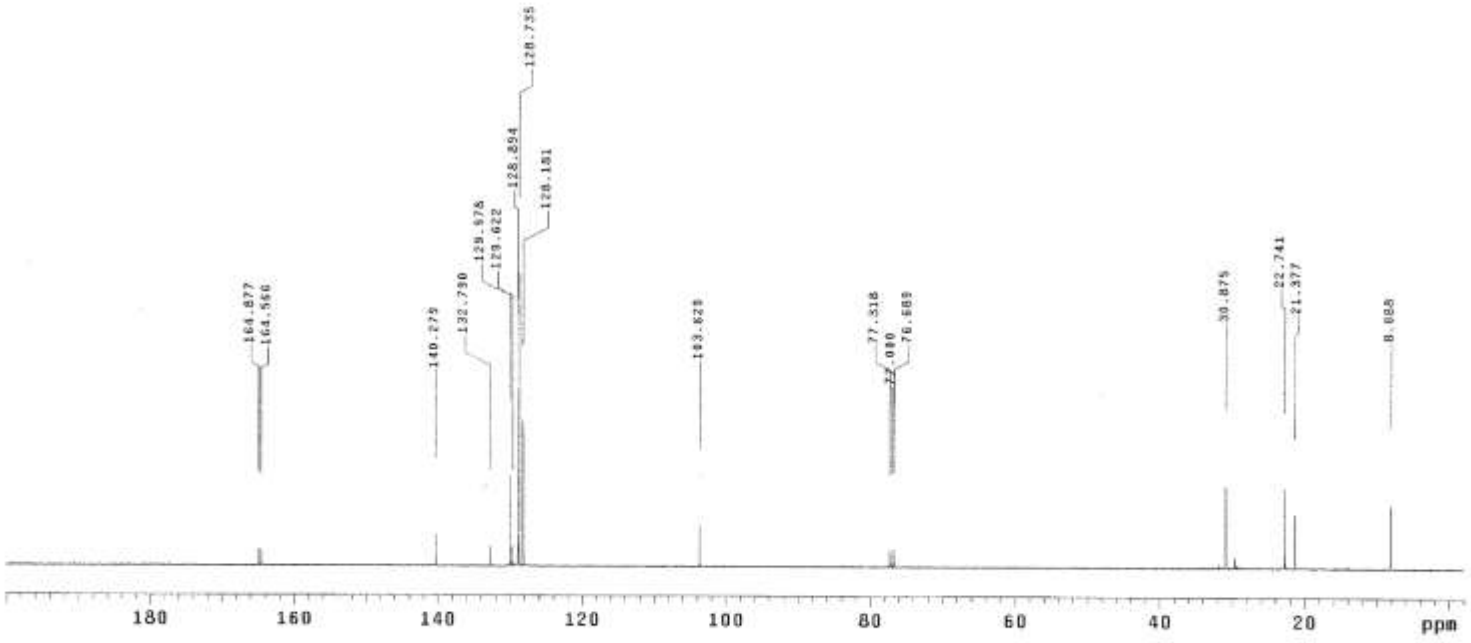


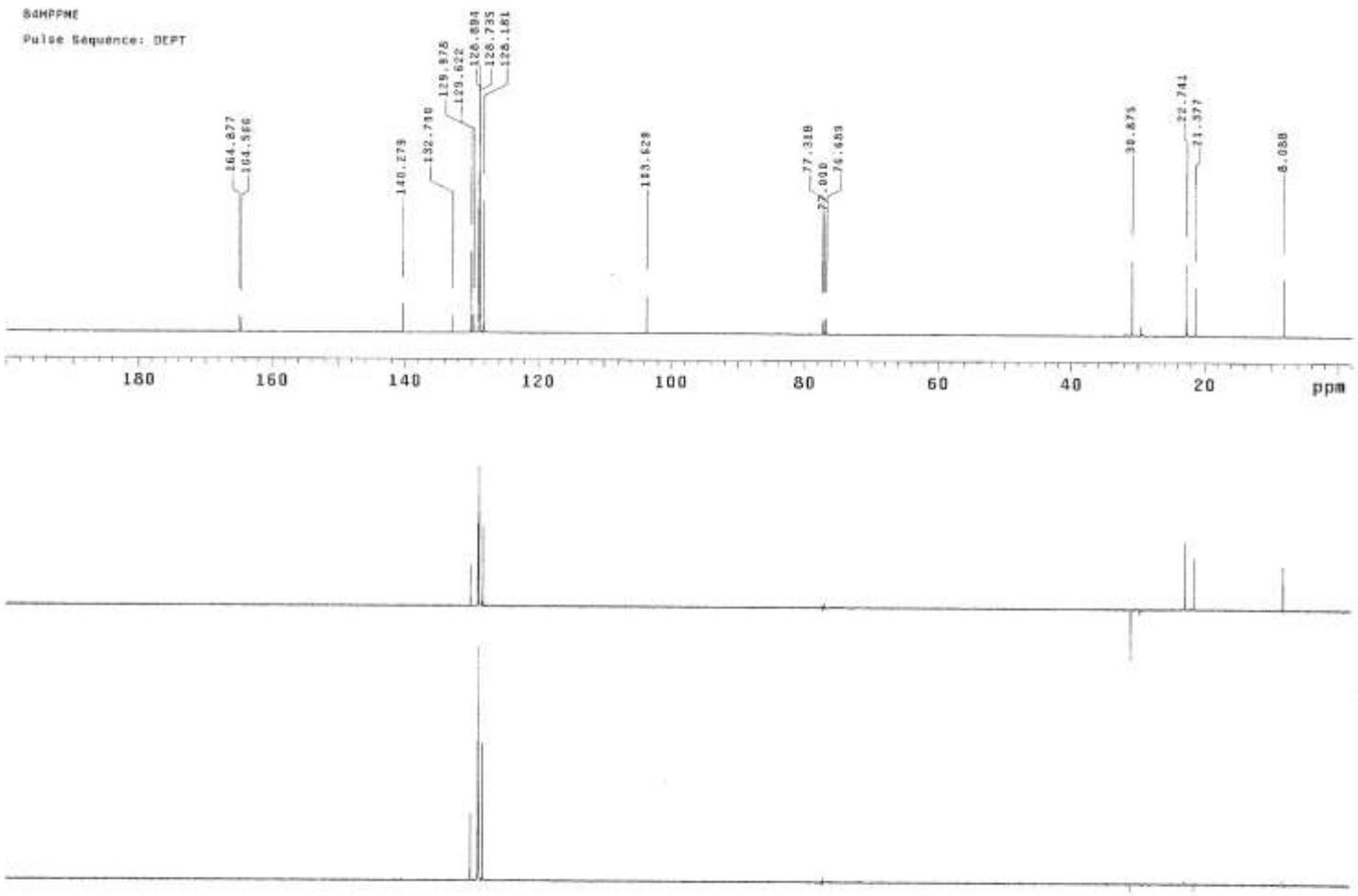


B6MPPME

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Nov 19 2014
Solvent: CDCl3
Ambient temperature
File: M02B2-14
Total 1256 repetitions

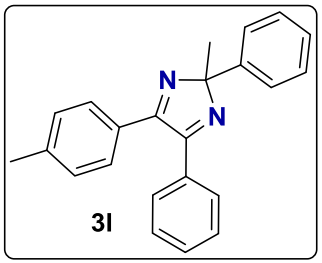



S6MPPME
Pulse Sequence: DEPT
164.877
164.586
140.279
132.798
129.878
129.622
128.804
128.735
128.181
113.628
77.318
77.000
76.683
30.875
22.741
21.377
8.088
180
160
140
120
100
80
60
40
20
ppm

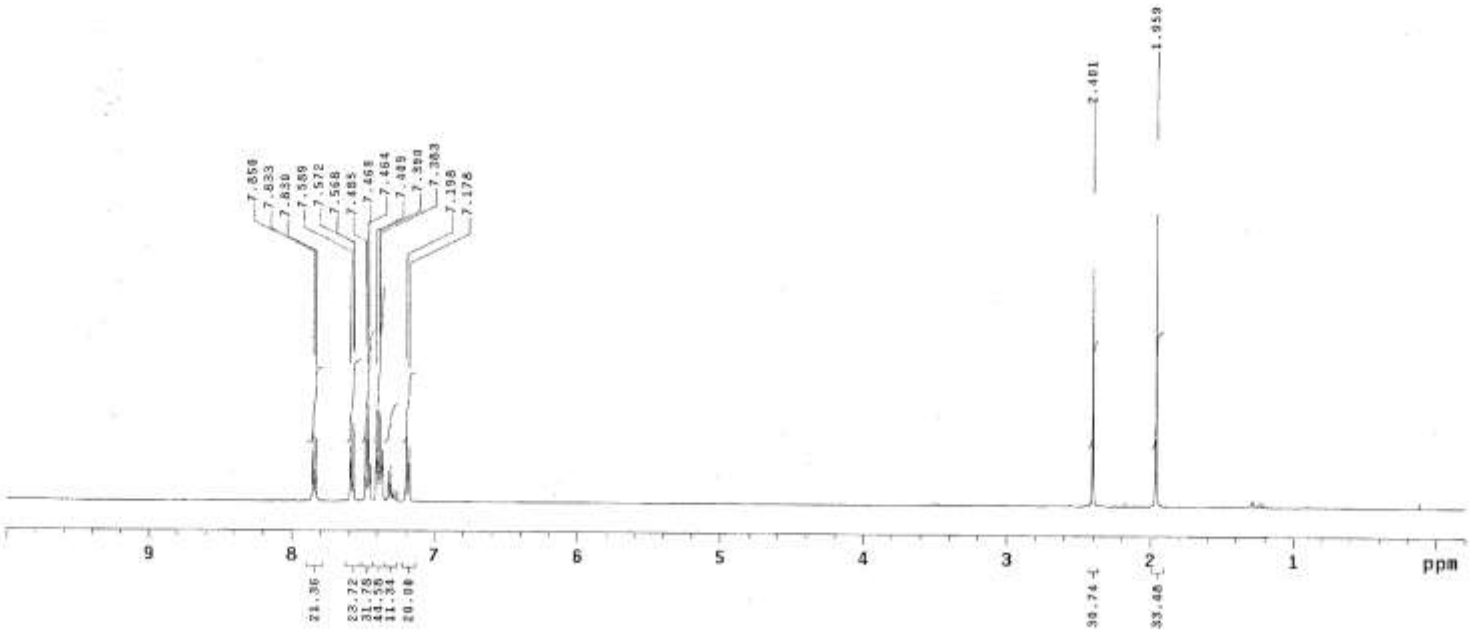
Hou-NB01-047

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Dec 11 2014
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



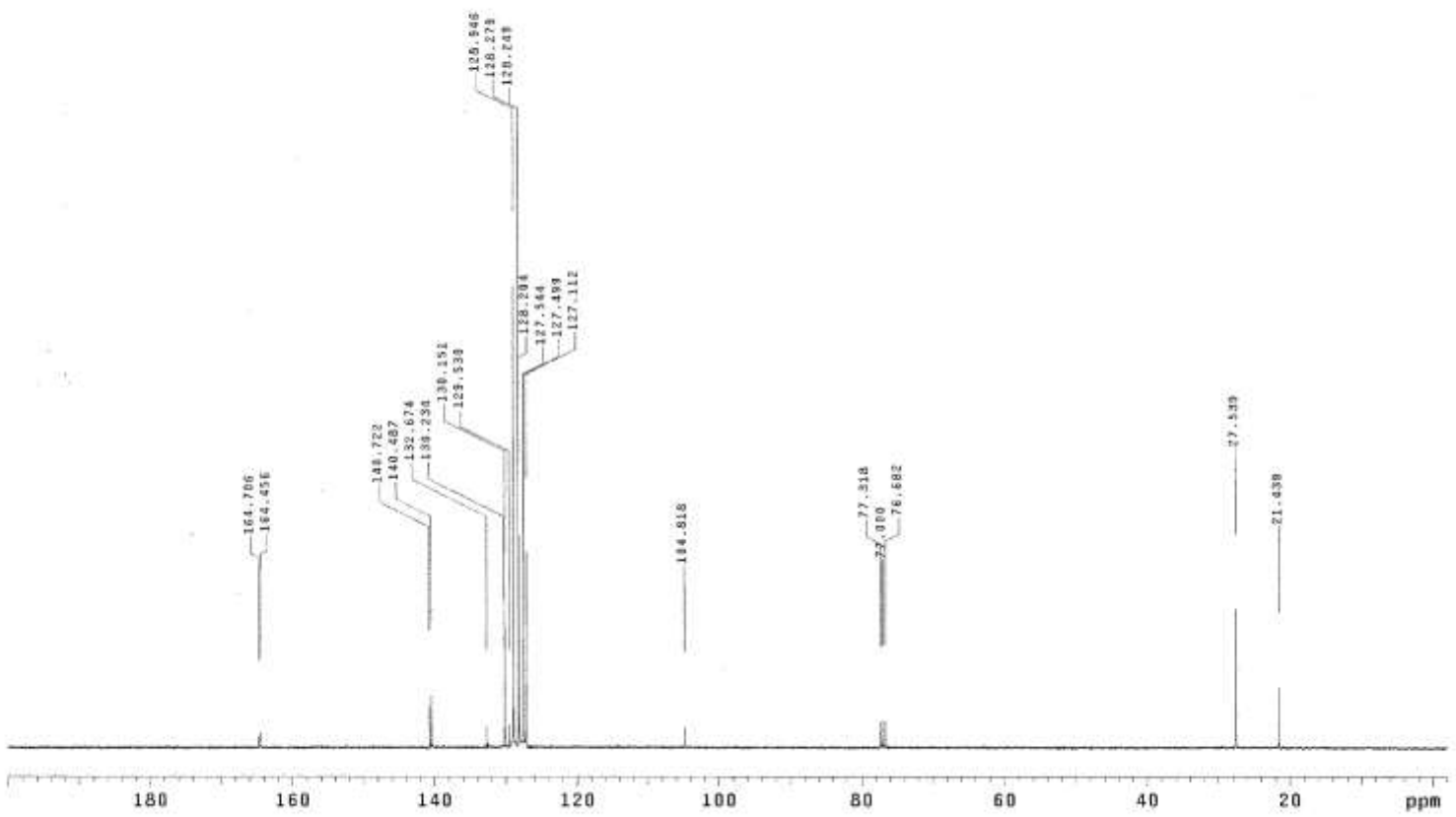
3l

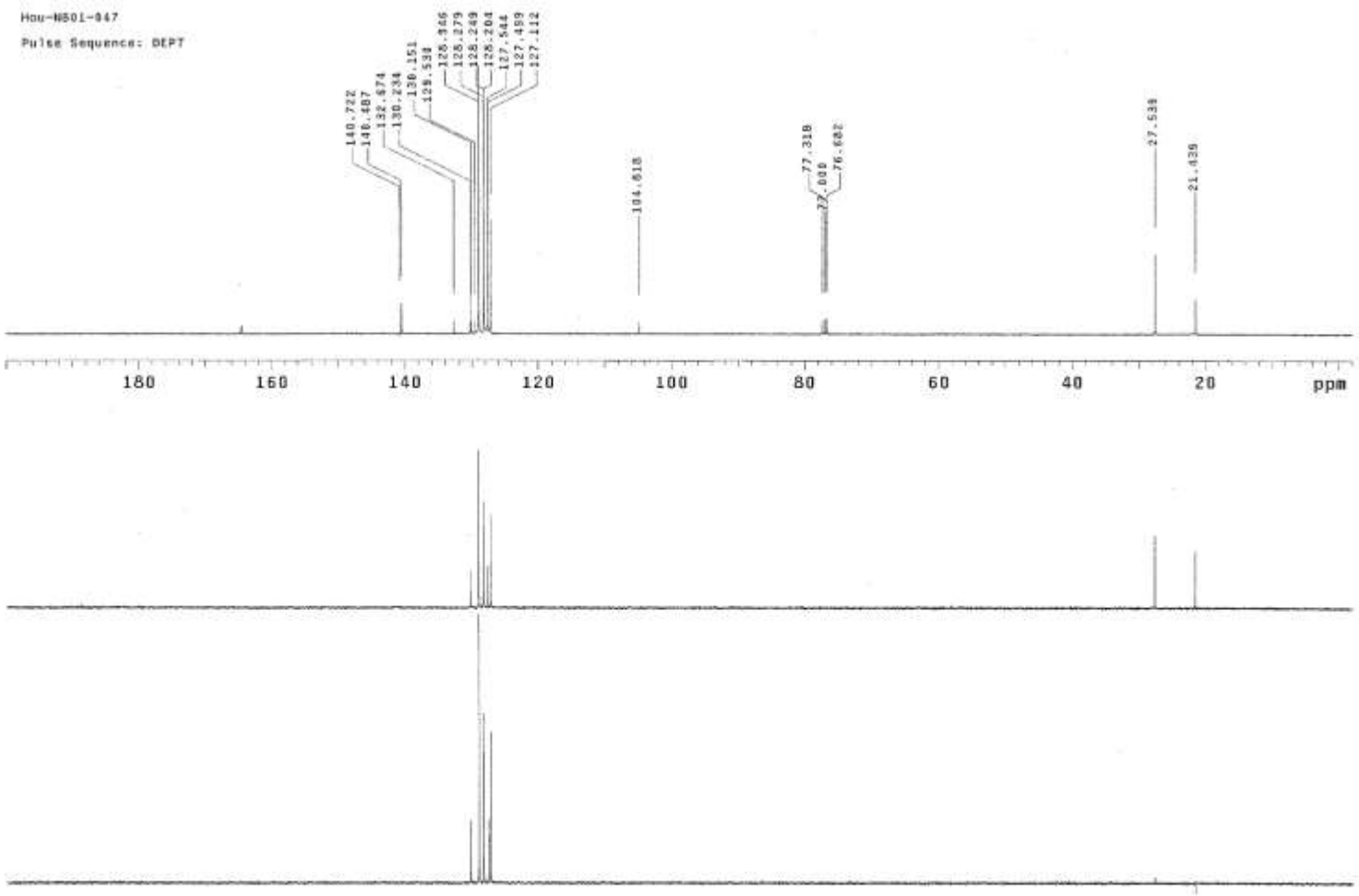


Hou-NB01-047

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Dec 11 2014
Solvent: CDCl3
Ambient temperature
Total 320 repetitions

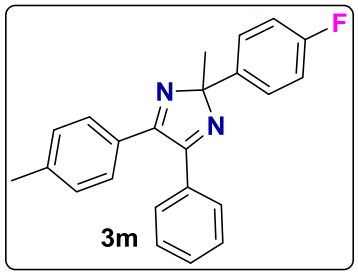


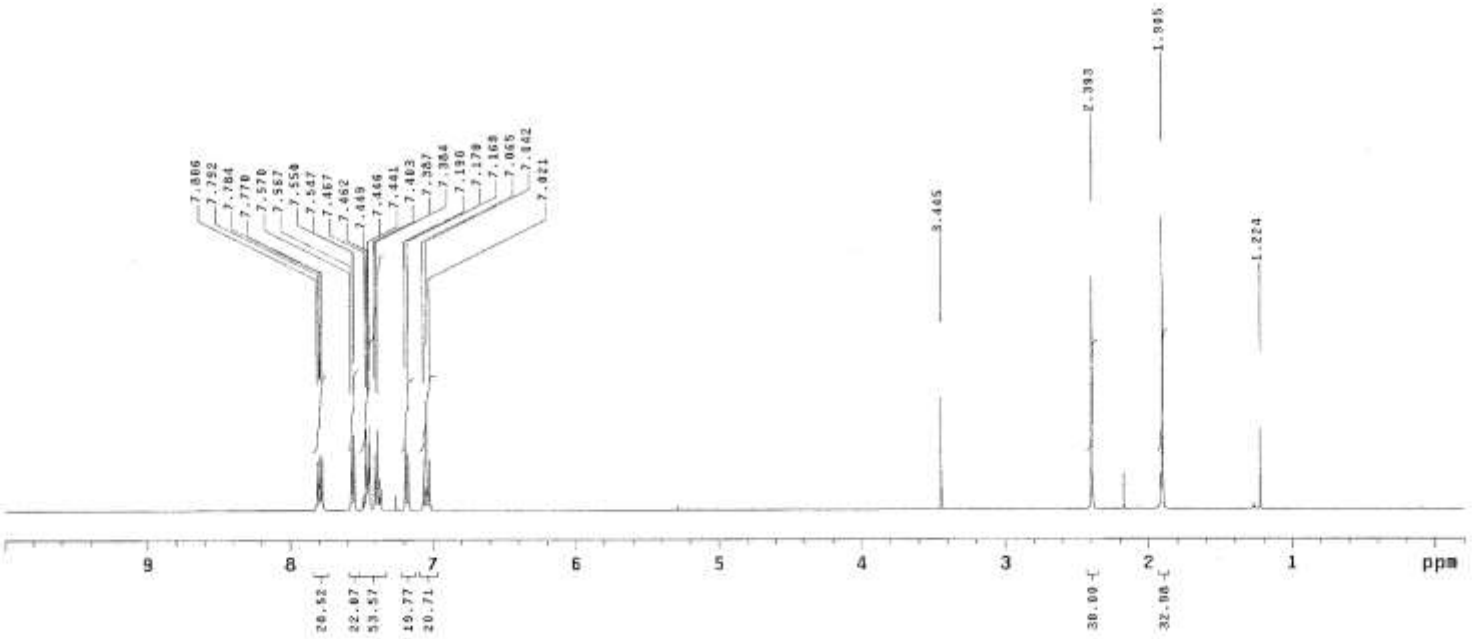

Hou-N801-047
Pulse Sequence: DEPT
140.722
140.487
132.674
130.234
130.151
129.538
128.966
128.279
128.249
128.204
127.544
127.459
127.112
104.618
77.318
77.000
76.682
27.538
21.439
180
160
140
120
100
80
60
40
20
ppm

B4MPPM4FP

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Nov 20 2014
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

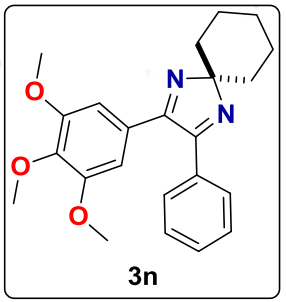




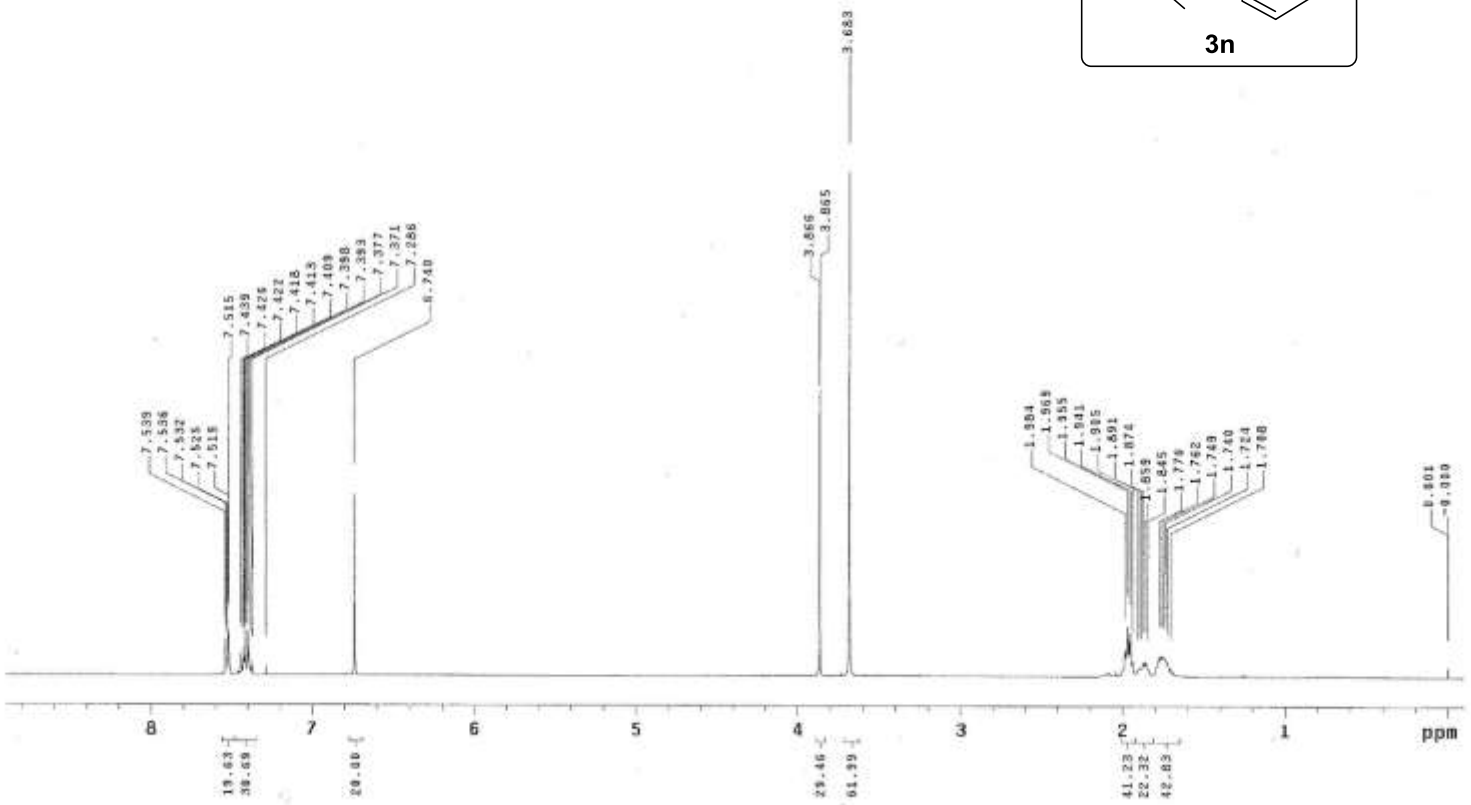
BMAPEM

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Apr 15 2014
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



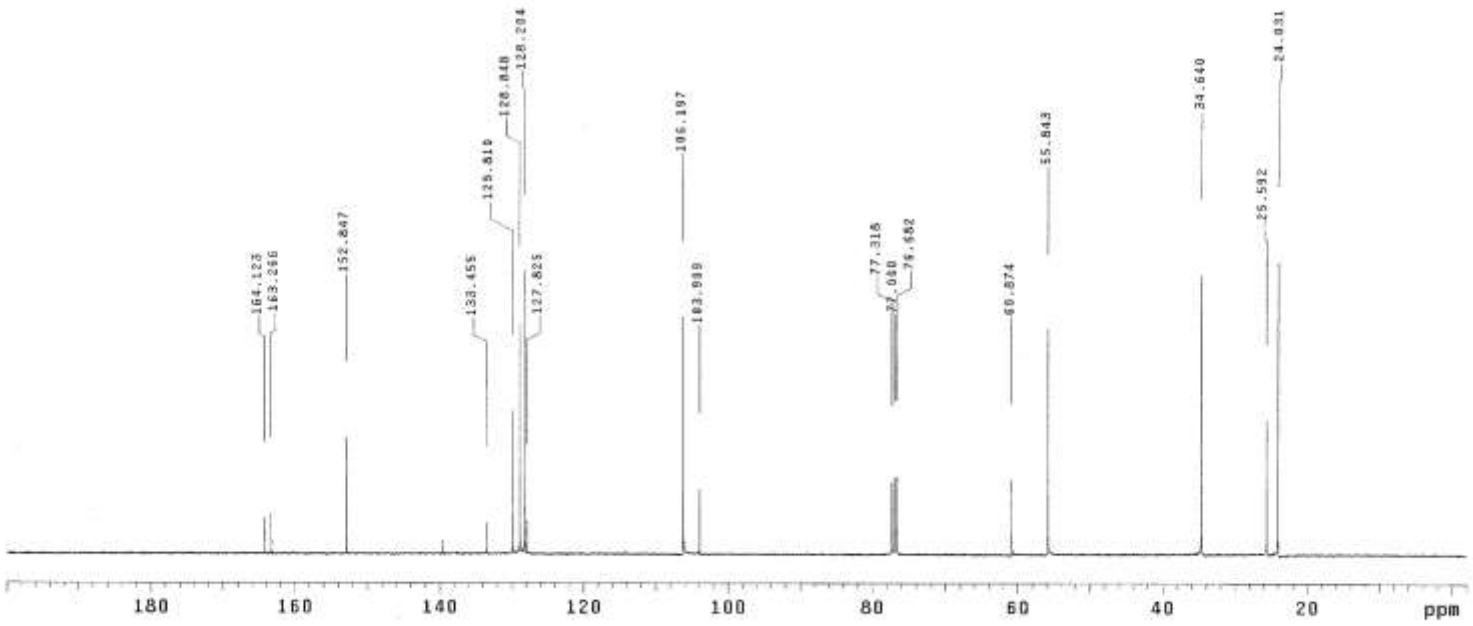
3n

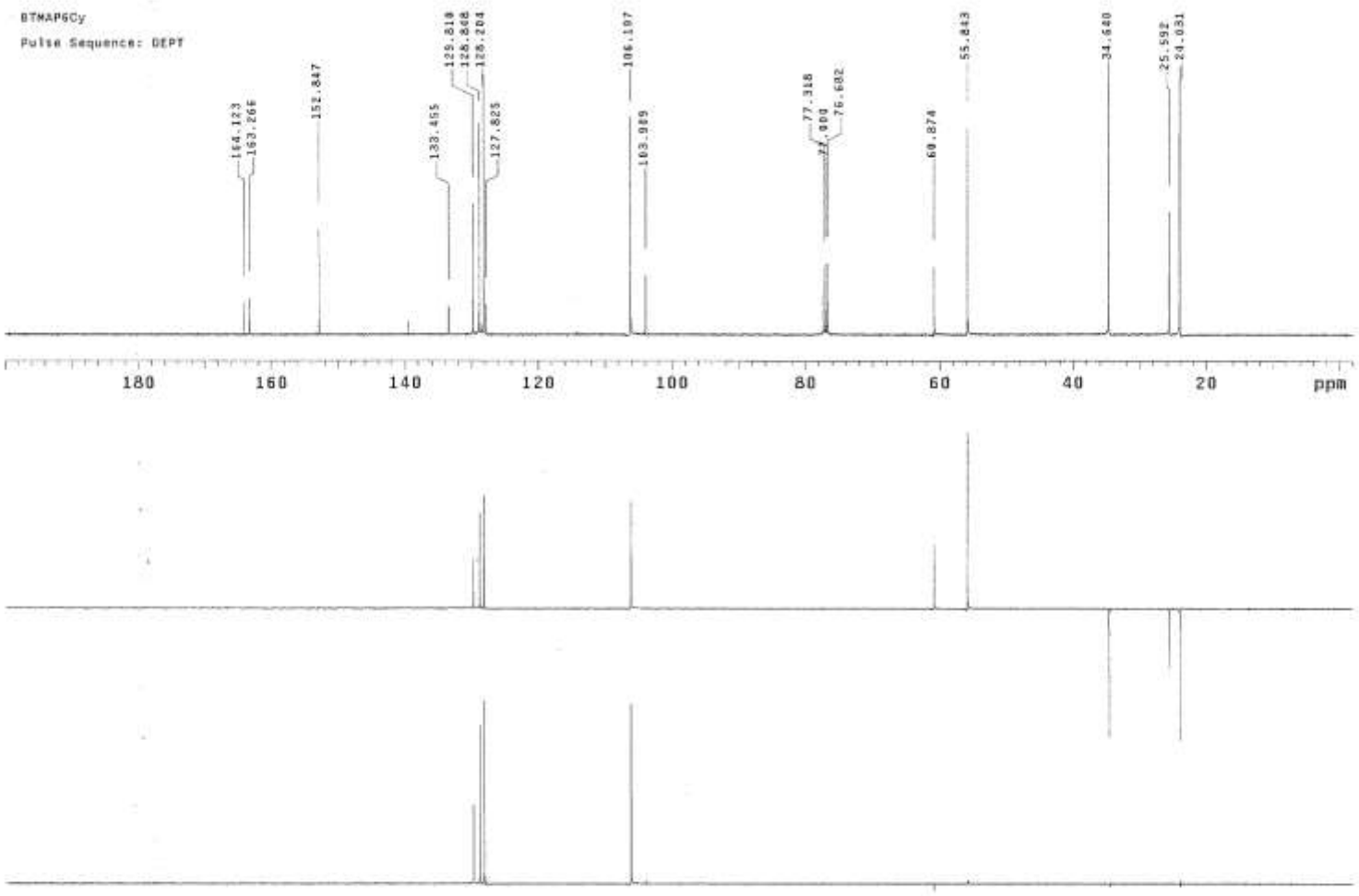


BTMAP6Cy

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Dec 12 2014
Solvent: CDCl3
Ambient temperature
Total 1856 repetitions

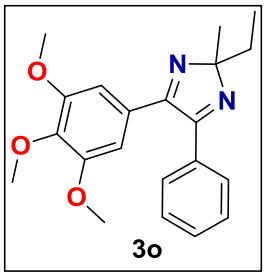



BTMAP6Cy
Pulse Sequence: DEPT
164.123
163.266
152.847
133.455
129.818
128.848
128.284
127.825
106.197
103.989
77.318
77.060
76.682
60.874
55.843
34.640
25.592
24.031
180
160
140
120
100
80
60
40
20
ppm

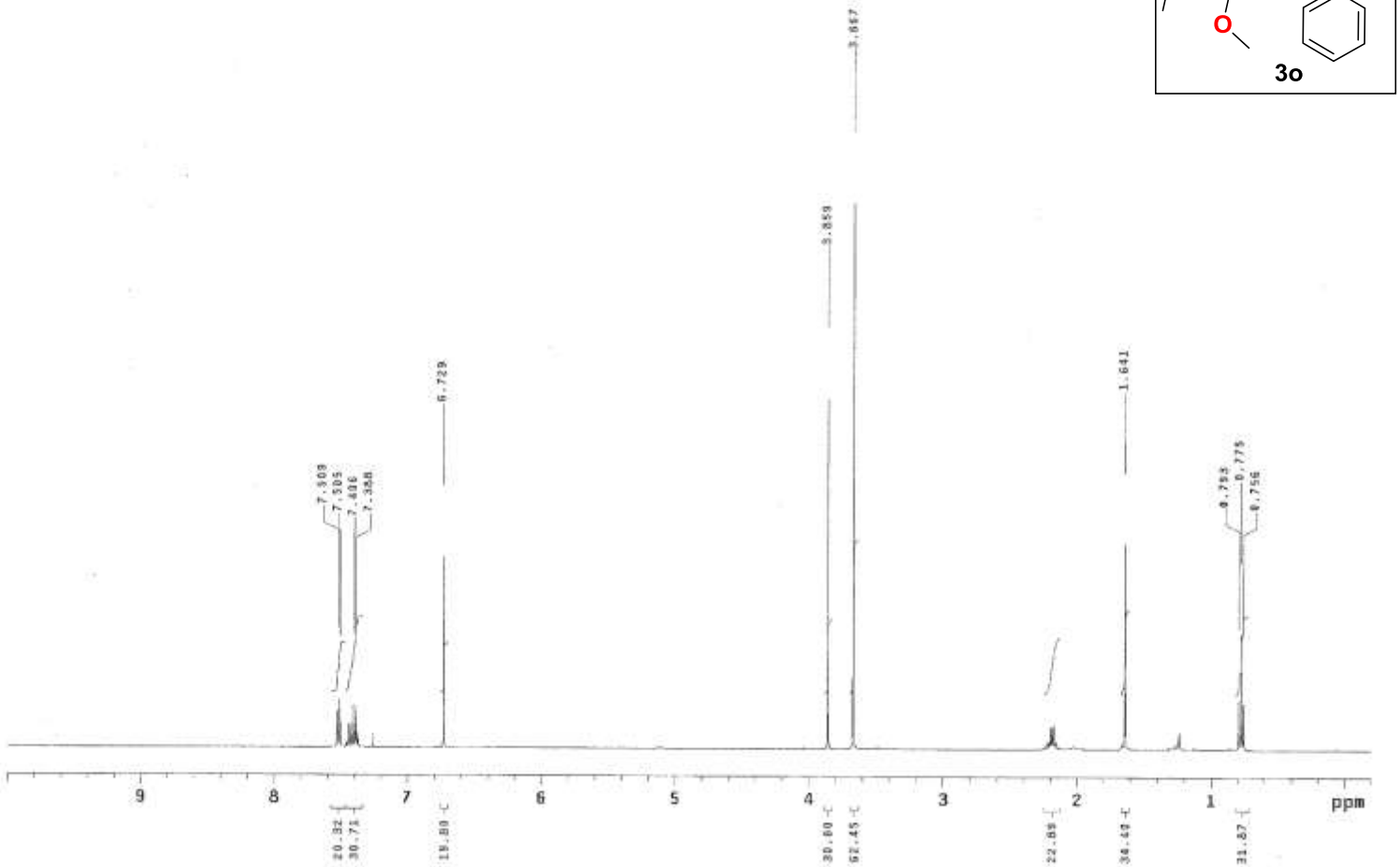
BTMAPME

Pulse Sequence: s2pul

Mercury=400BB "MercuryPlus400"
Date: Nov 19 2014
Solvent: CDCl3
Ambient temperature
File: M0282-4
Total 32 repetitions



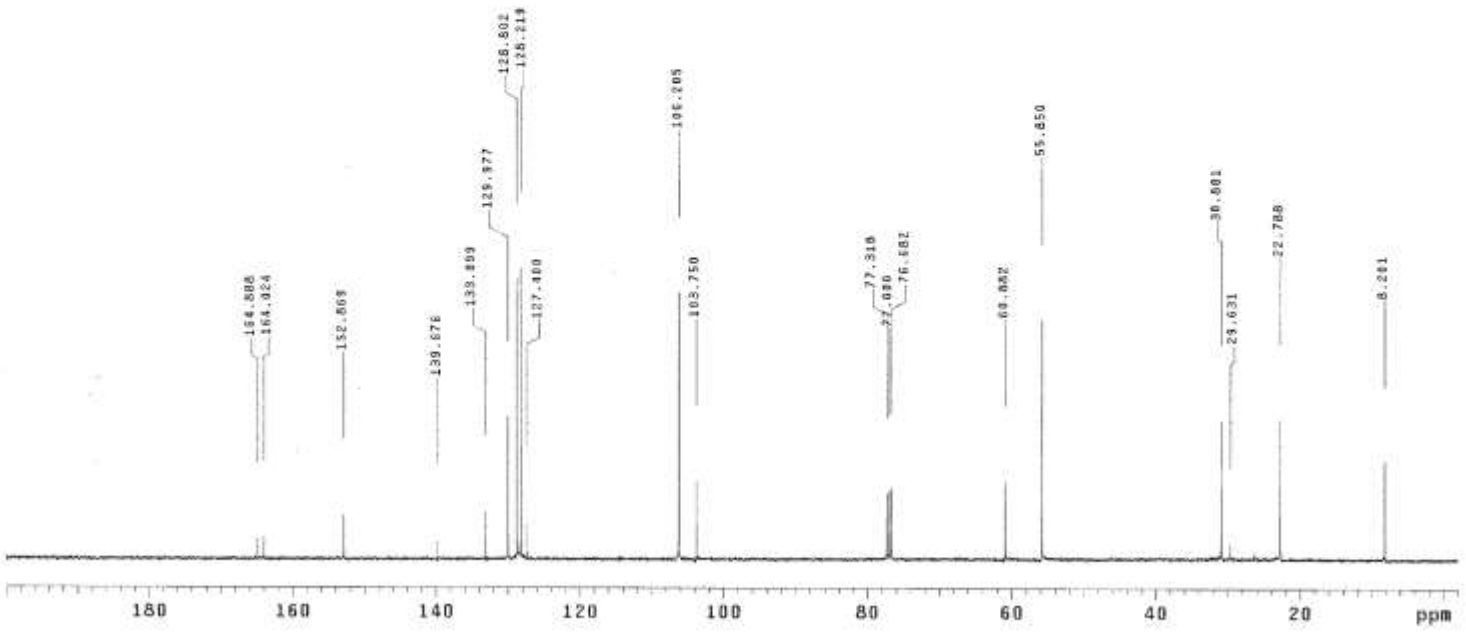
3o

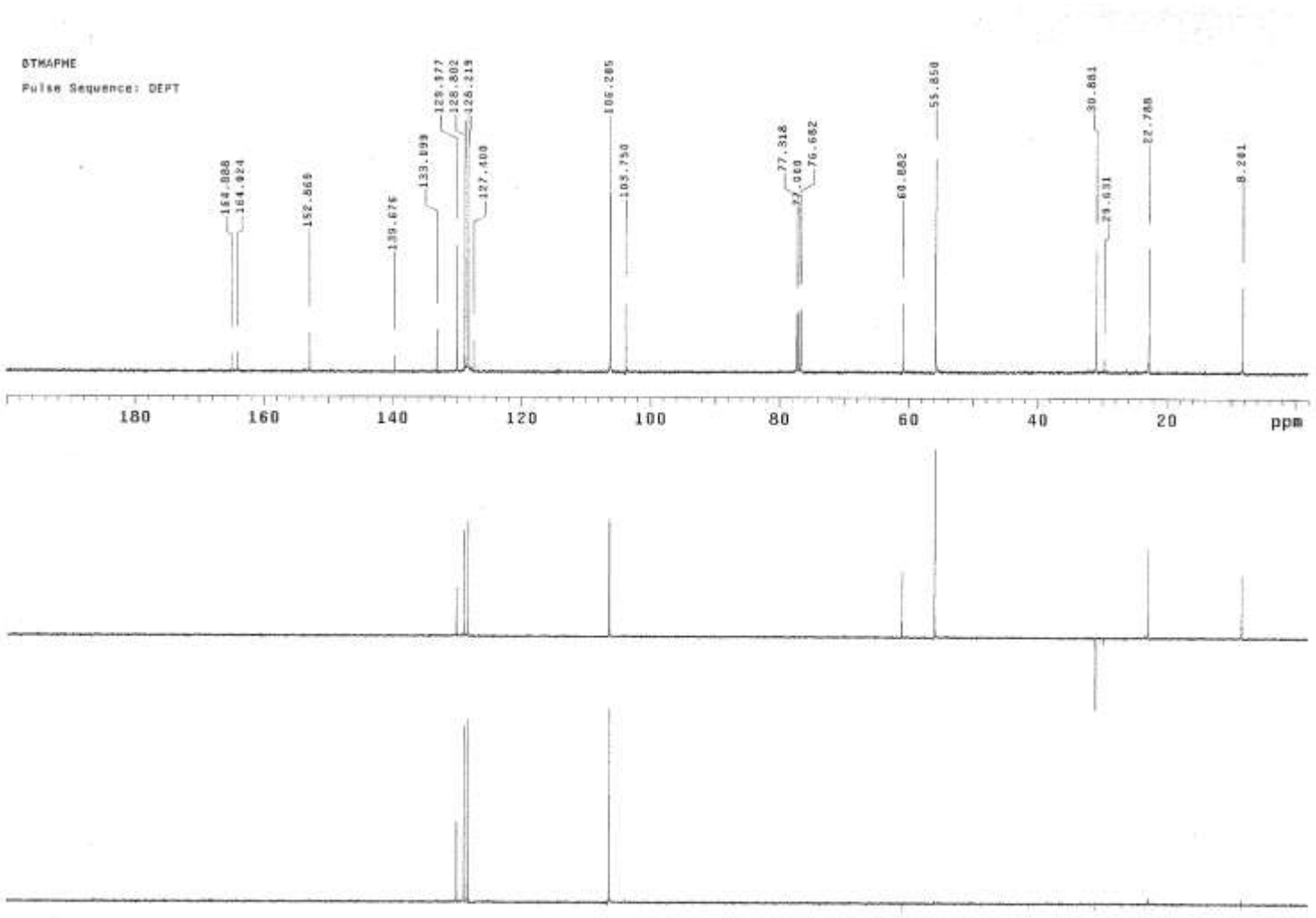


BTMAPME

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Nov 19 2014
Solvent: CDCl3
Ambient temperature
File: MD282-5
Total 64000 repetitions

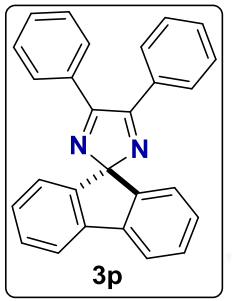



DTKAPHE
Pulse Sequence: DEFT
164.888
164.924
152.869
139.676
133.099
129.377
128.802
128.219
127.400
106.285
105.750
77.318
77.060
76.682
60.882
55.850
30.881
29.631
22.788
8.281
180
160
140
120
100
80
60
40
20
ppm

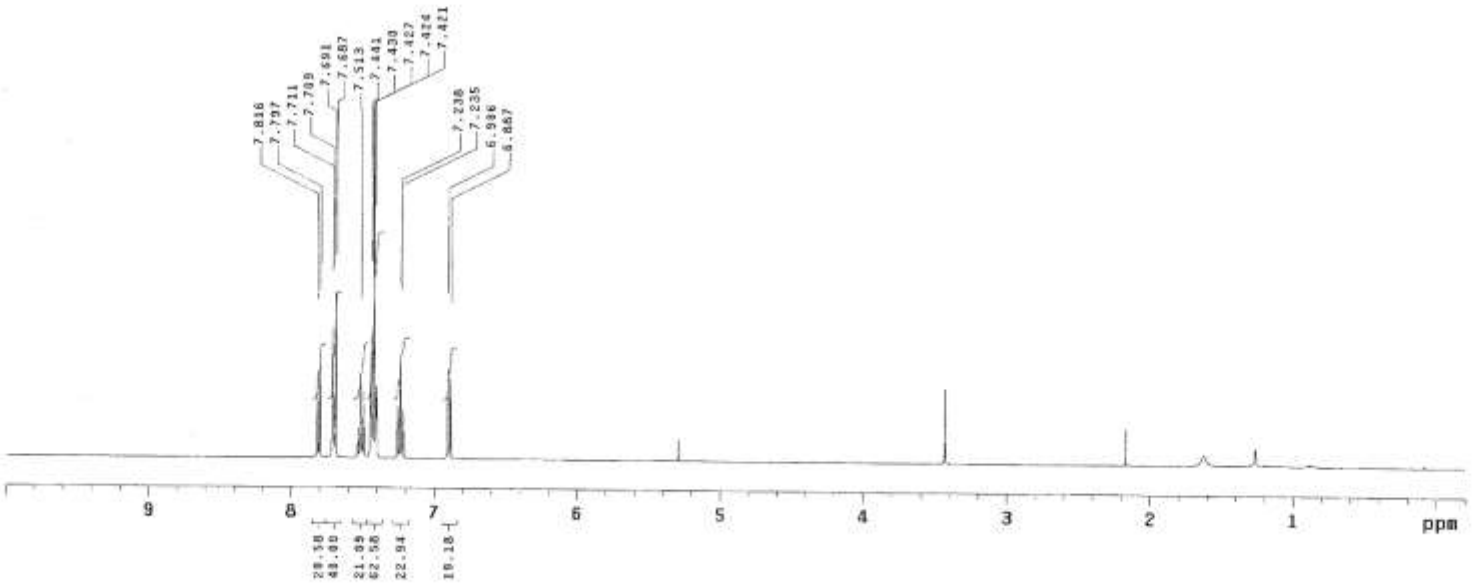
8PP9-F

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Nov 28 2014
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



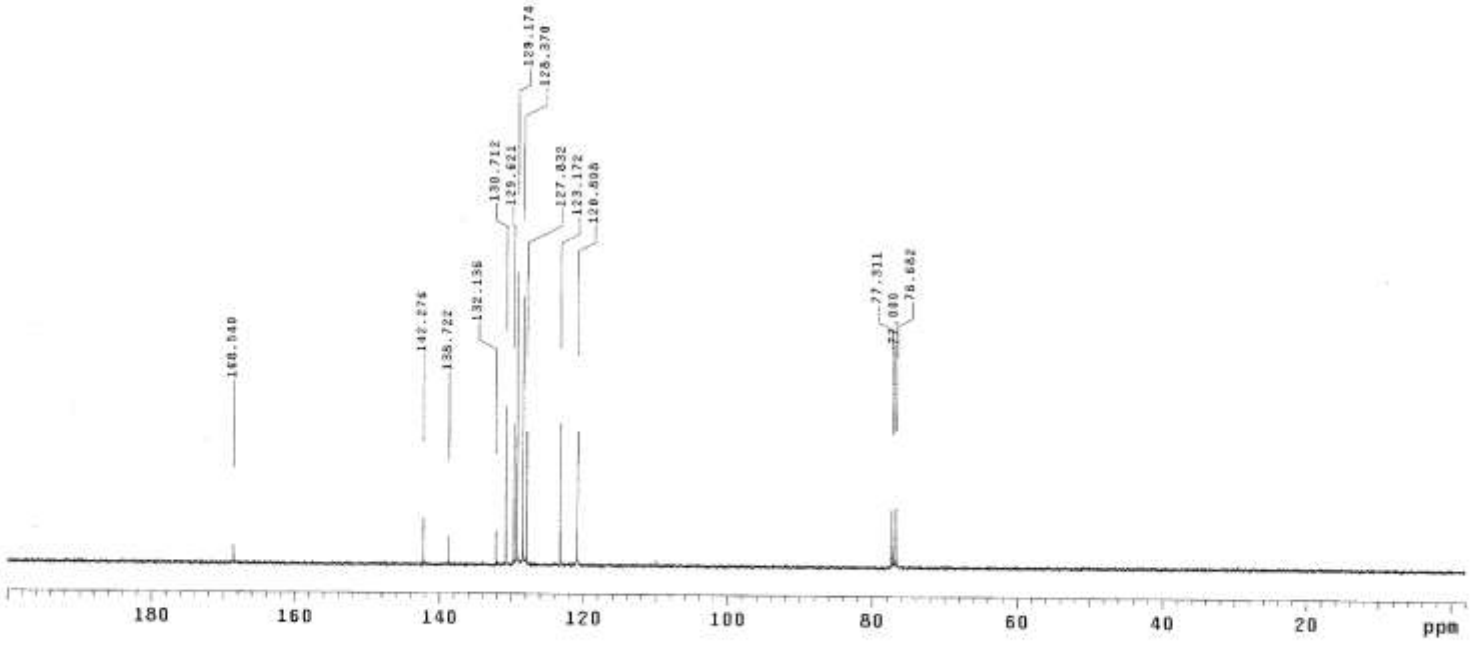
3p

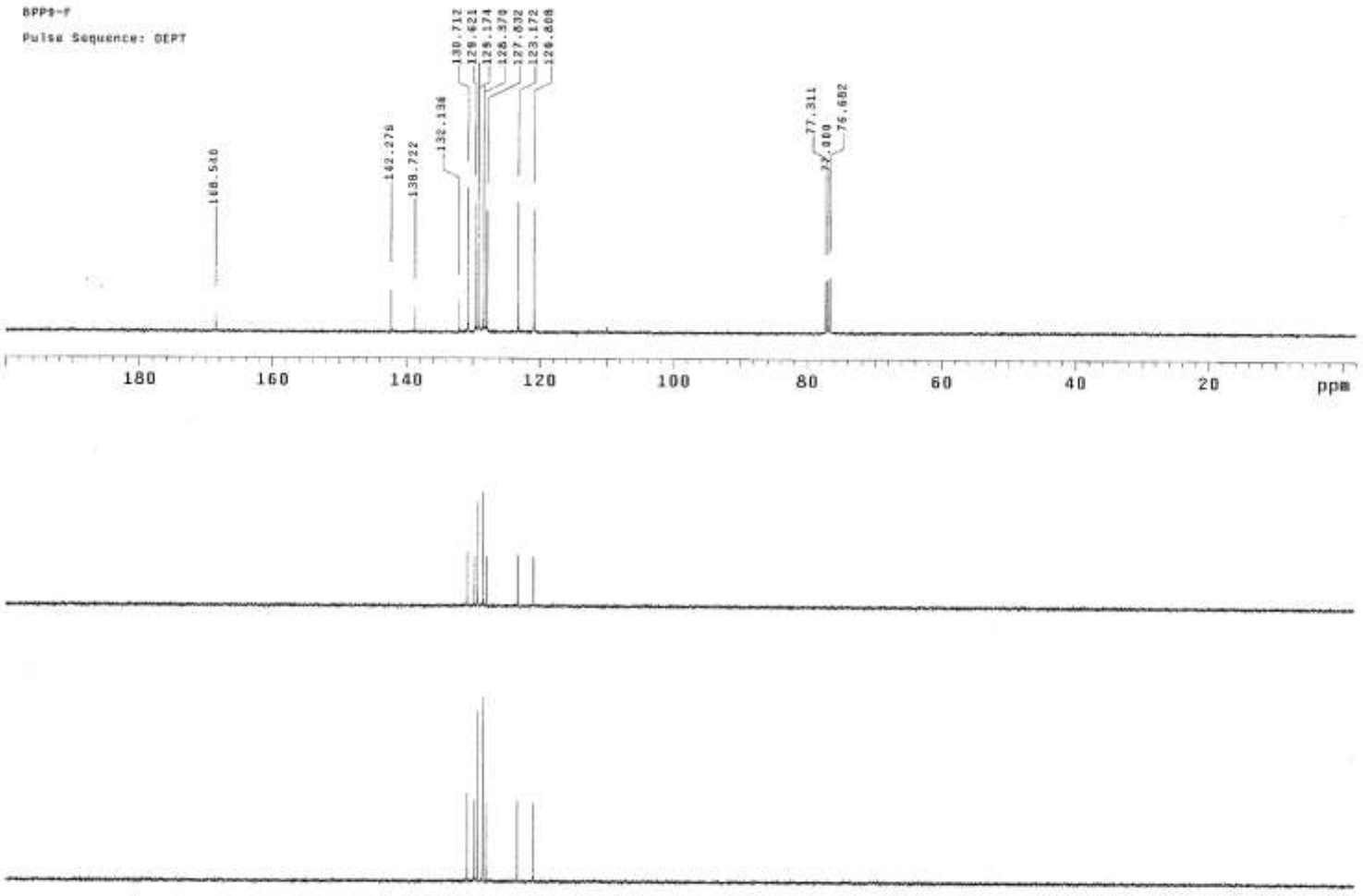


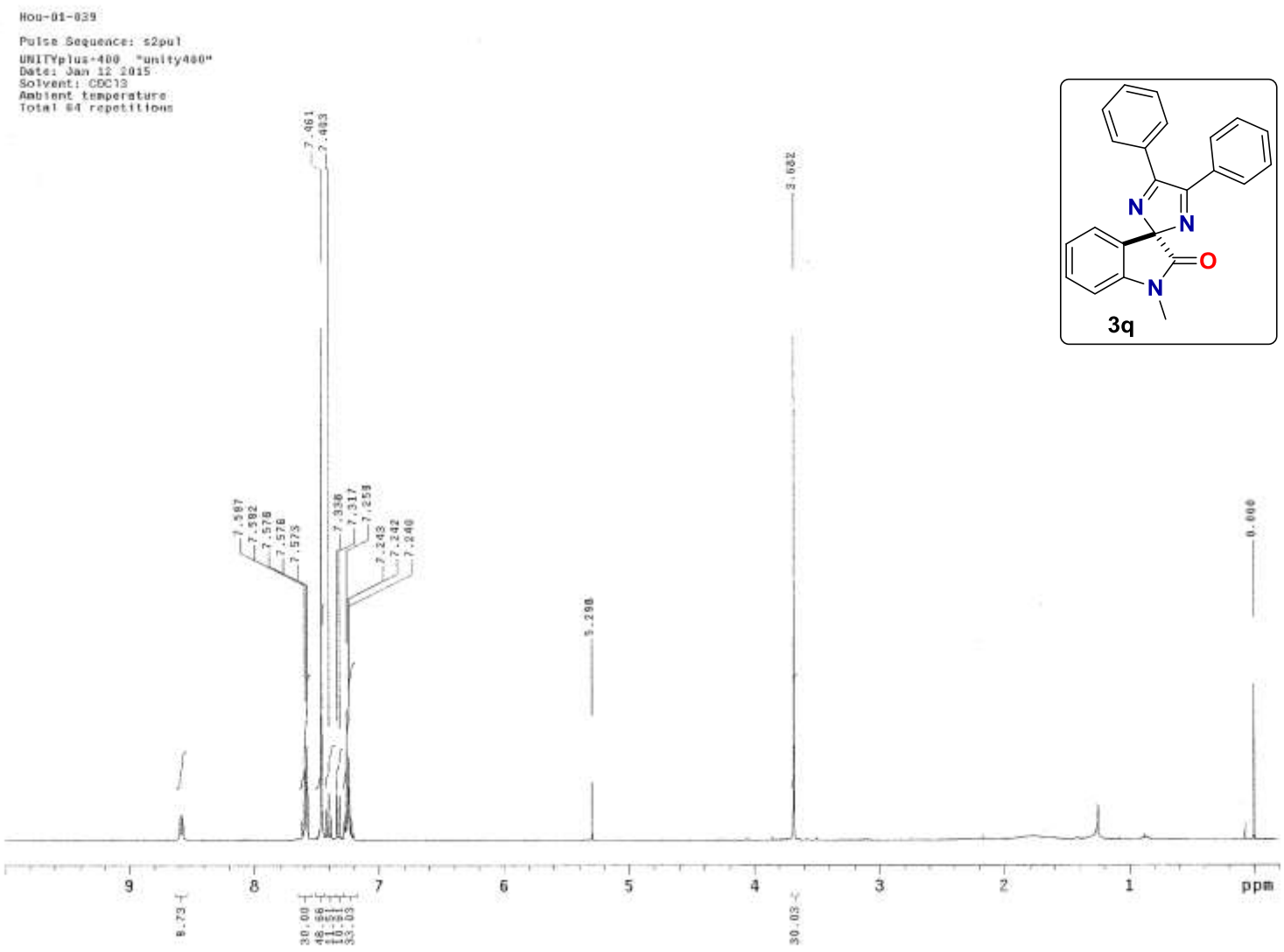
BPPS-F

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Nov 20 2014
Solvent: CDCl3
Ambient temperature
Total 512 repetitions



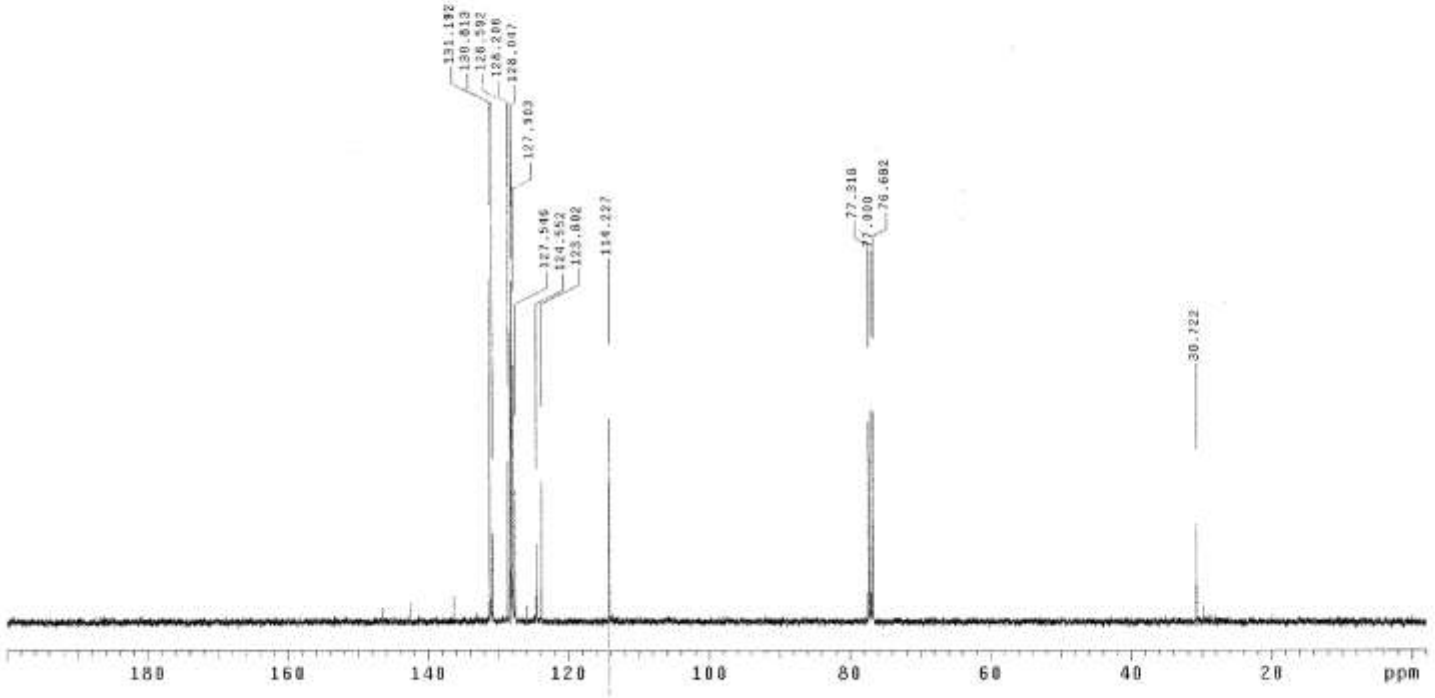

BPP9-F
Pulse Sequence: DEPT
168.516
142.276
138.722
132.138
130.712
129.621
129.174
128.579
127.632
123.172
120.808
77.311
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm

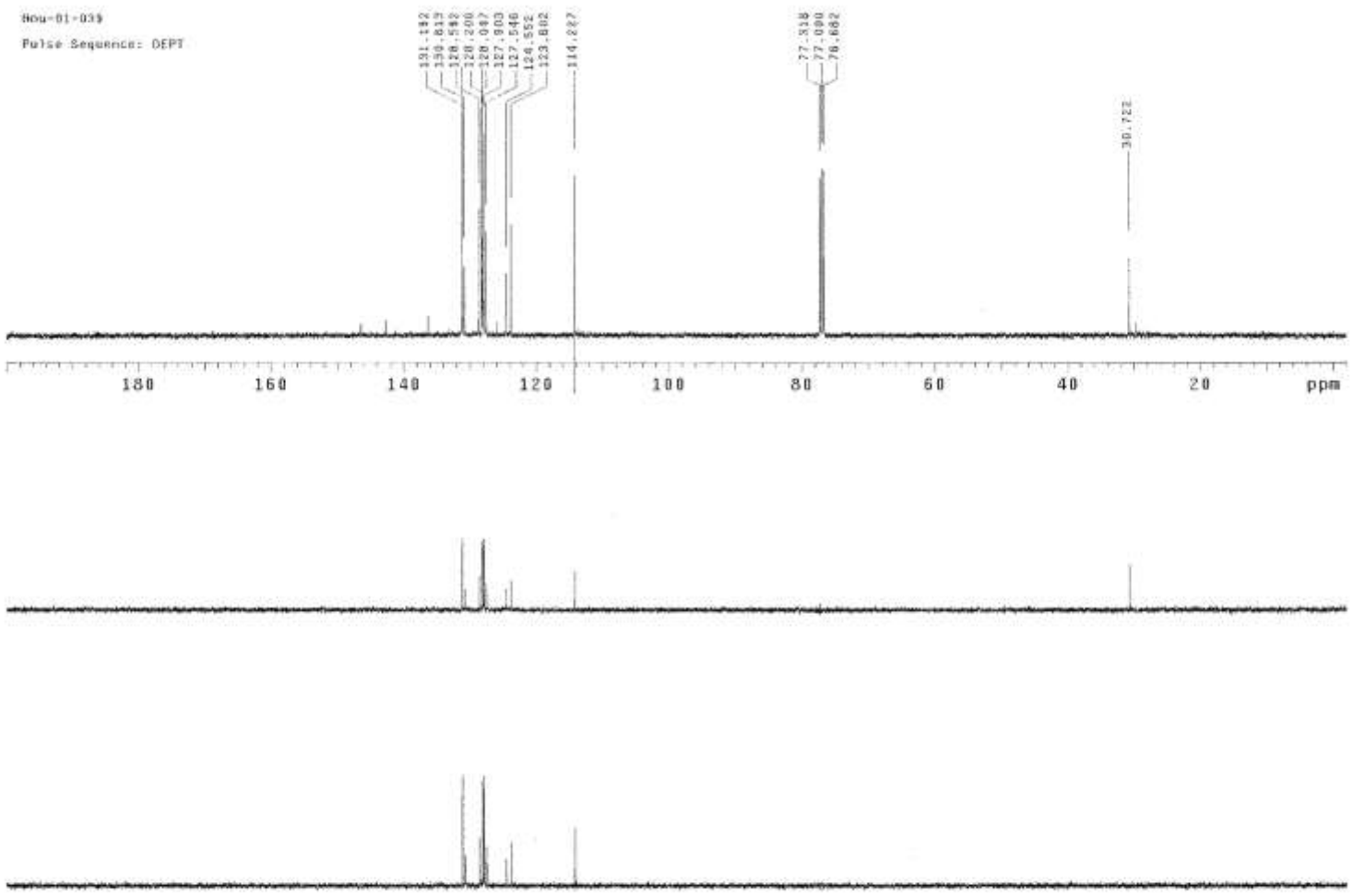

Hou-01-039
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 12 2015
Solvent: CDCl3
Ambient temperature
Total 64 repetitions
7.461
7.463
3.682
7.587
7.582
7.578
7.576
7.573
7.336
7.317
7.253
7.243
7.242
7.240
5.298
0.000
N
N
O
N
3q
9
8
7
6
5
4
3
2
1
ppm
8.73
30.00
48.86
11.51
10.03
33.03
30.03

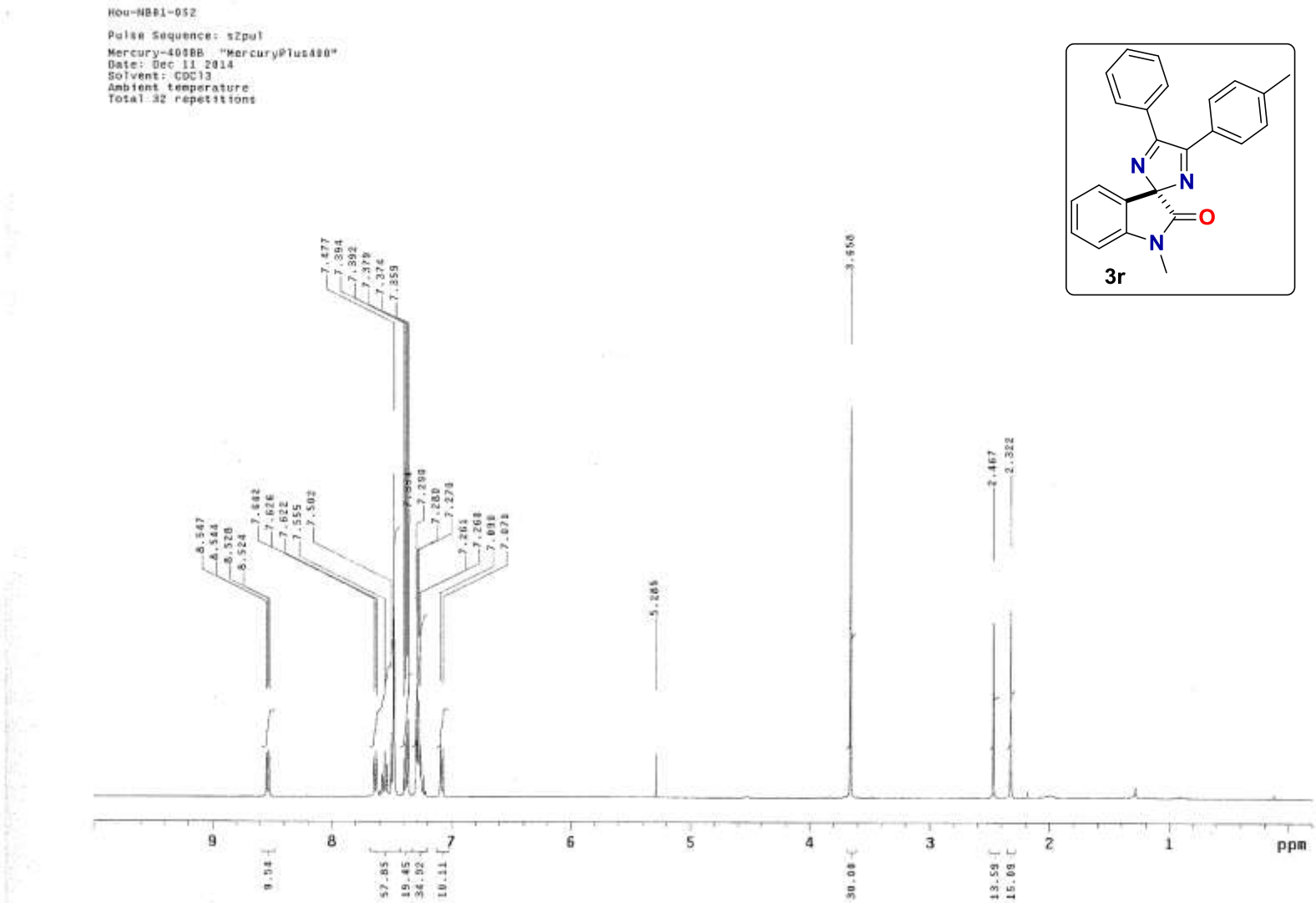
Mou-01-039

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 12 2015
Solvent: CDCl3
Ambient temperature
Total 14096 repetitions



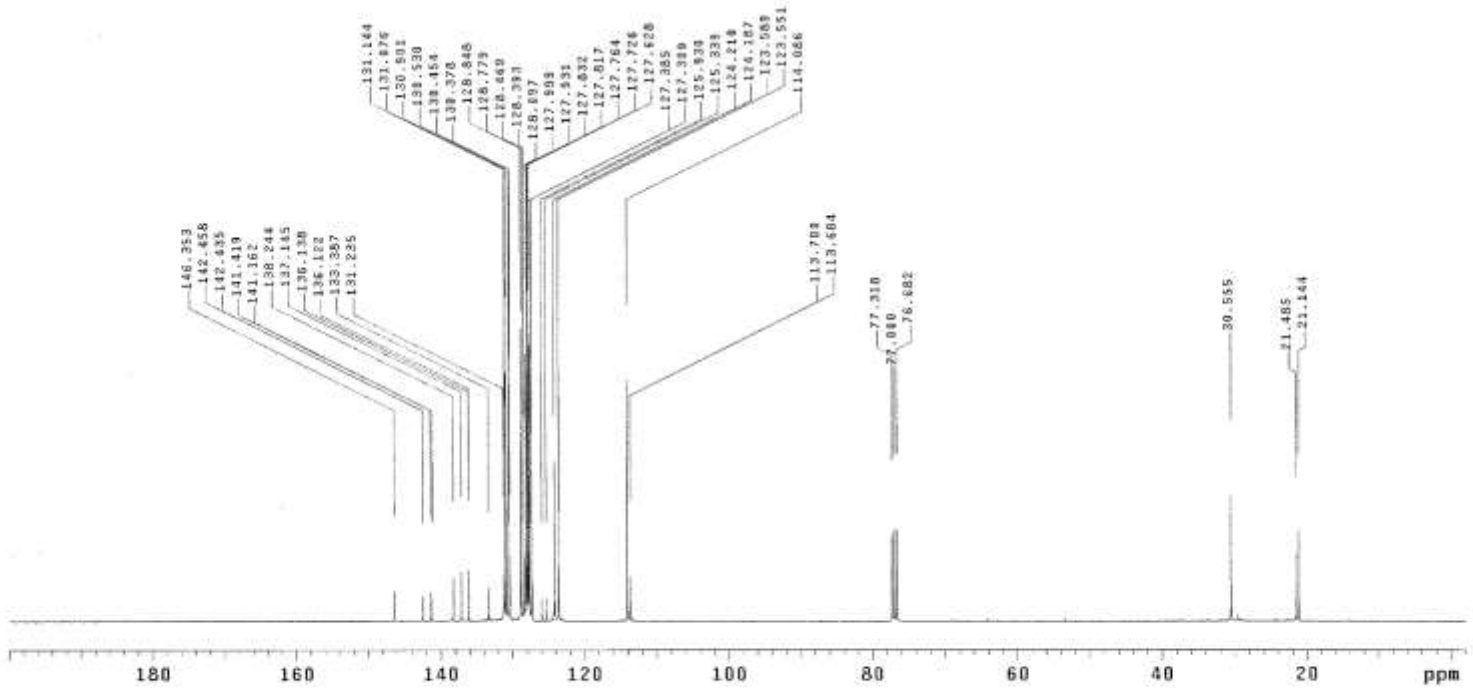

Hou-01-039
Pulse Sequence: DEPT
131.182
130.819
128.582
128.200
128.087
127.903
127.646
124.552
123.802
114.287
77.318
77.000
76.682
30.722
180
160
140
120
100
80
60
40
20
ppm

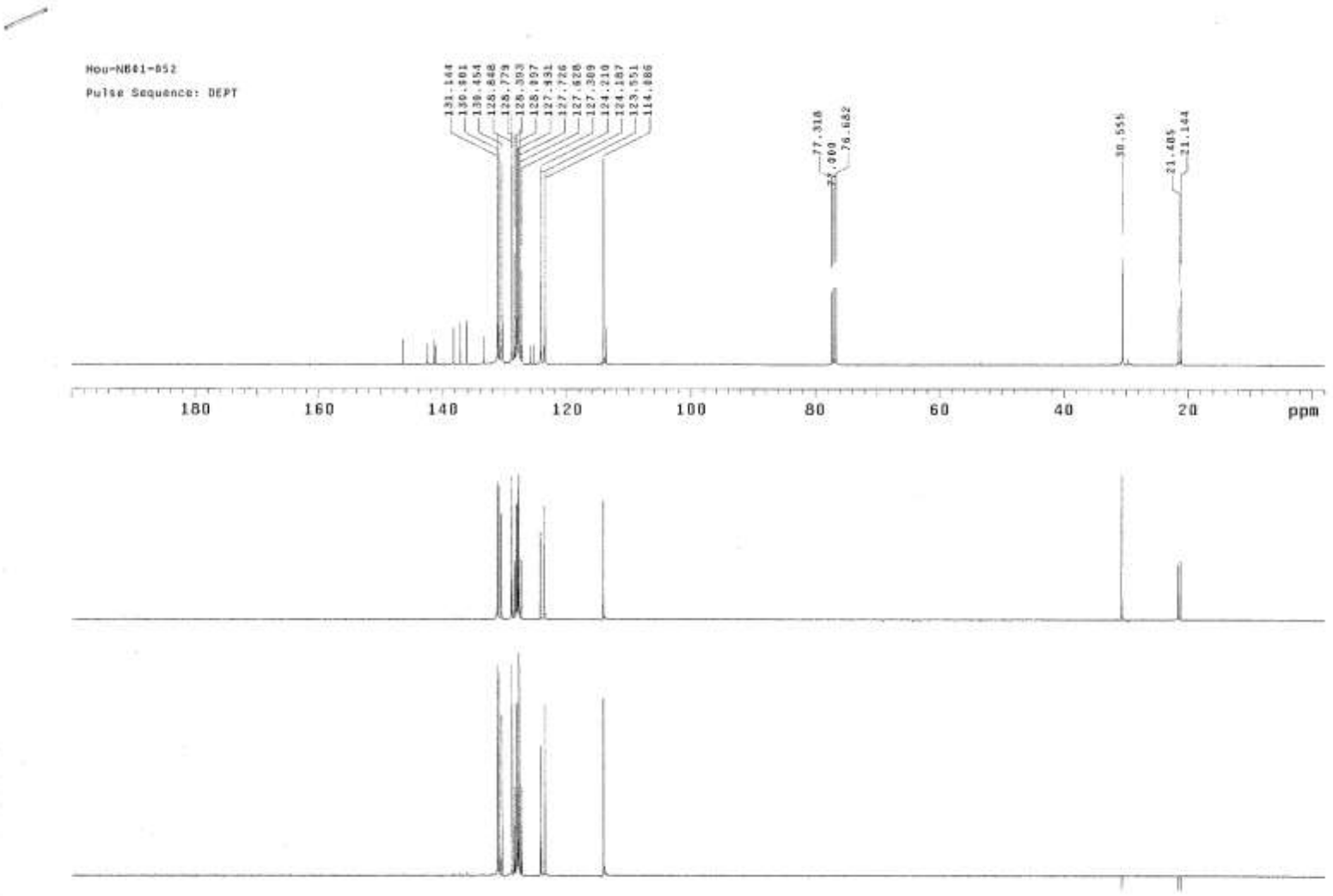

Hou-NB01-052
Pulse Sequence: s2pul
Mercury-400BB "Mercury@Tus400"
Date: Dec 11 2014
Solvent: CDCl3
Ambient temperature
Total 32 repetitions
3r
ppm

Hou-N801-052

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Dec 11 2014
Solvent: CDCl3
Ambient temperature
Total 12800 repetitions

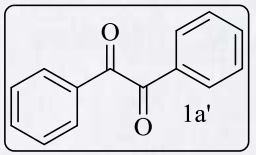



Hou-NB01-052
Pulse Sequence: DEPT
131.144
130.601
130.454
128.848
128.779
128.393
128.097
127.931
127.726
127.628
127.389
124.210
124.187
123.551
114.886
77.318
77.000
76.682
30.555
21.405
21.144
180
160
140
120
100
80
60
40
20
ppm

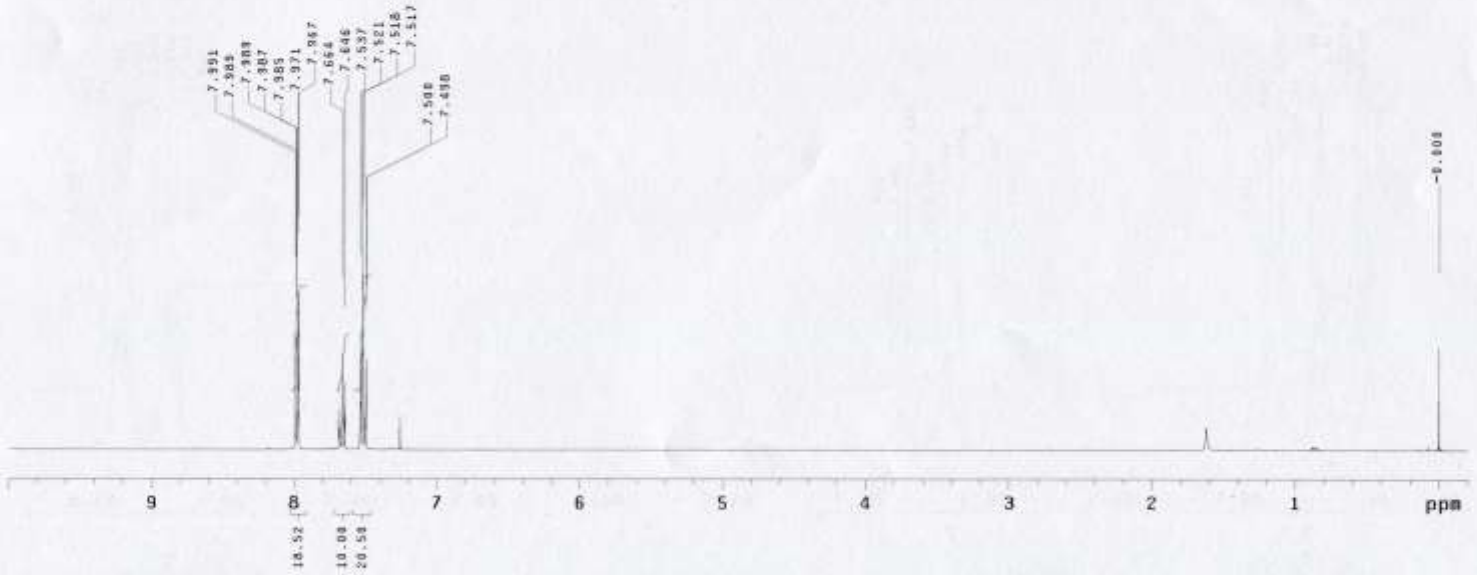
Balar-Inf-1

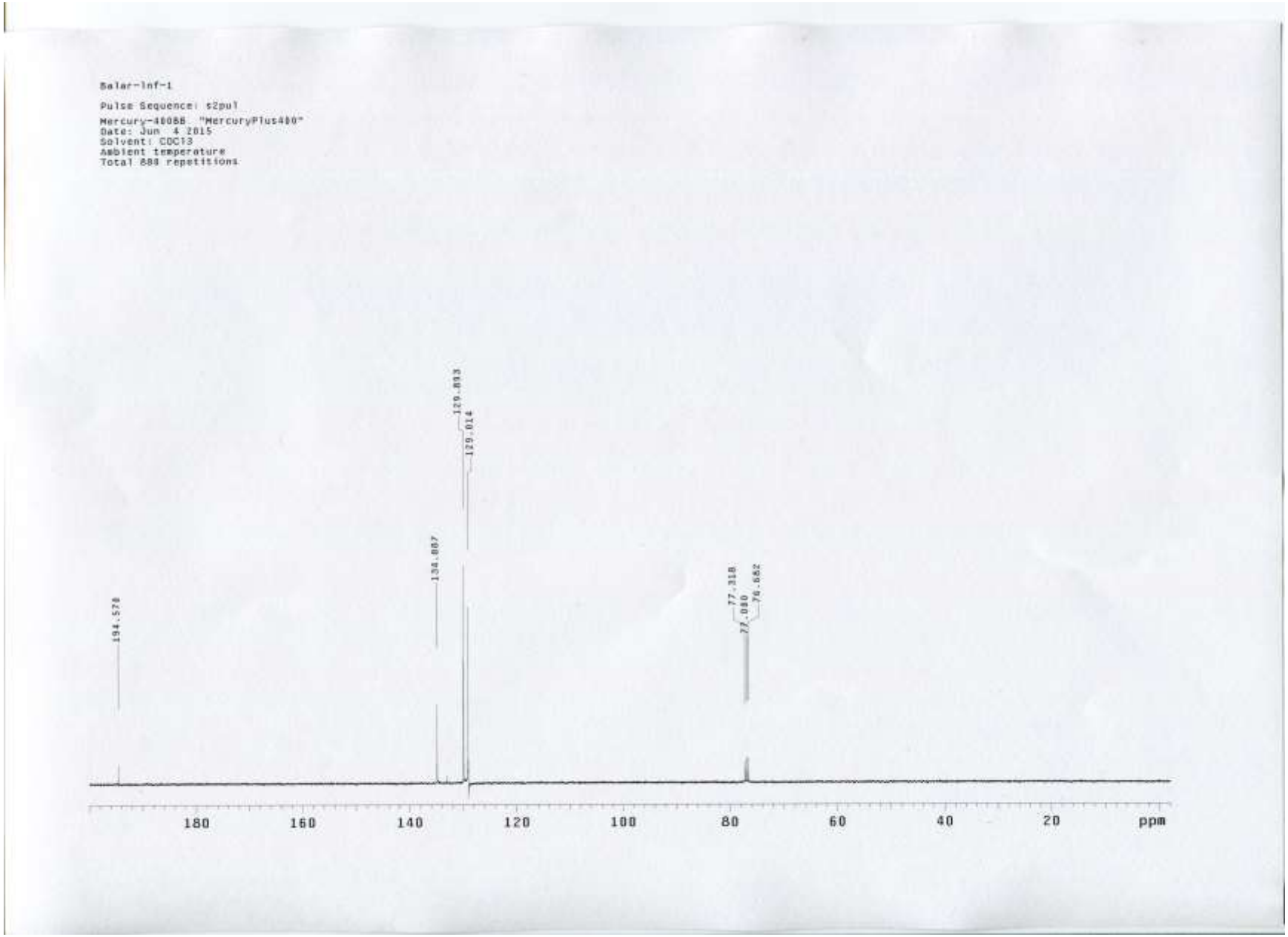
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jun 4 2015
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



1a'




Balar-Inf-1
Pulse Sequence: s2pul
Mercury-400BB "MercuryPlus400"
Date: Jun 4 2015
Solvent: CDCl3
Ambient temperature
Total 888 repetitions
194.578
134.887
129.893
129.014
77.318
77.060
76.682
180
160
140
120
100
80
60
40
20
ppm

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: hou0155

```
Bond precision:  C-C = 0.0058 A          Wavelength=0.71073

Cell:            a=10.6396(6)     b=10.6396(6)     c=13.8377(8)
                 alpha=90         beta=90          gamma=90
Temperature:     284 K
```

	Calculated	Reported
Volume	1566.4(2)	1566.44(15)
Space group	I 41	I 41
Hall group	I 4bw	?
Moiety formula	C17 H16 N2	C17 H16 N2
Sum formula	C17 H16 N2	C17 H16 N2
Mr	248.32	248.32
Dx,g cm-3	1.053	1.053
Z	4	4
Mu (mm-1)	0.062	0.062
F000	528.0	528.0
F000'	528.17	
h,k,lmax	13,13,17	13,13,17
Nref	1603[836]	1604
Tmin,Tmax	0.979,0.985	0.971,0.985
Tmin'	0.971	

```
Correction method= # Reported T Limits: Tmin=0.971 Tmax=0.985
AbsCorr = MULTI-SCAN

Data completeness= 1.92/1.00      Theta(max)= 26.290

R(reflections)= 0.0689( 1427)     wR2(reflections)= 0.2158( 1604)

S = 1.066                 Npar= 88
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
STRVA01_ALERT_2_C           Chirality of atom sites is inverted?
          From the CIF: _refine_ls_abs_structure_Flack    1.000
          From the CIF: _refine_ls_abs_structure_Flack_su    8.000
PLAT031_ALERT_4_C Refined Extinction Parameter within Range ......      2.500 Sigma
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       3.09 Report
PLAT213_ALERT_2_C Atom C9              has ADP max/min Ratio .....        3.1 prolat
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        3.8 Ratio
PLAT222_ALERT_3_C Large Non-Solvent  H     Uiso(max)/Uiso(min) ...        4.3 Ratio
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....         C8 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.5 Note
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0058 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C8     -   C9     ...       1.66 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C8     -   C9_a   ...       1.66 Ang.
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .      8.000 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.14 Report
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...          5 Units
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for     C8     Check
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   7 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 21/04/2015; check.def file version of 09/03/2015

Datablock hou0155 - ellipsoid plot

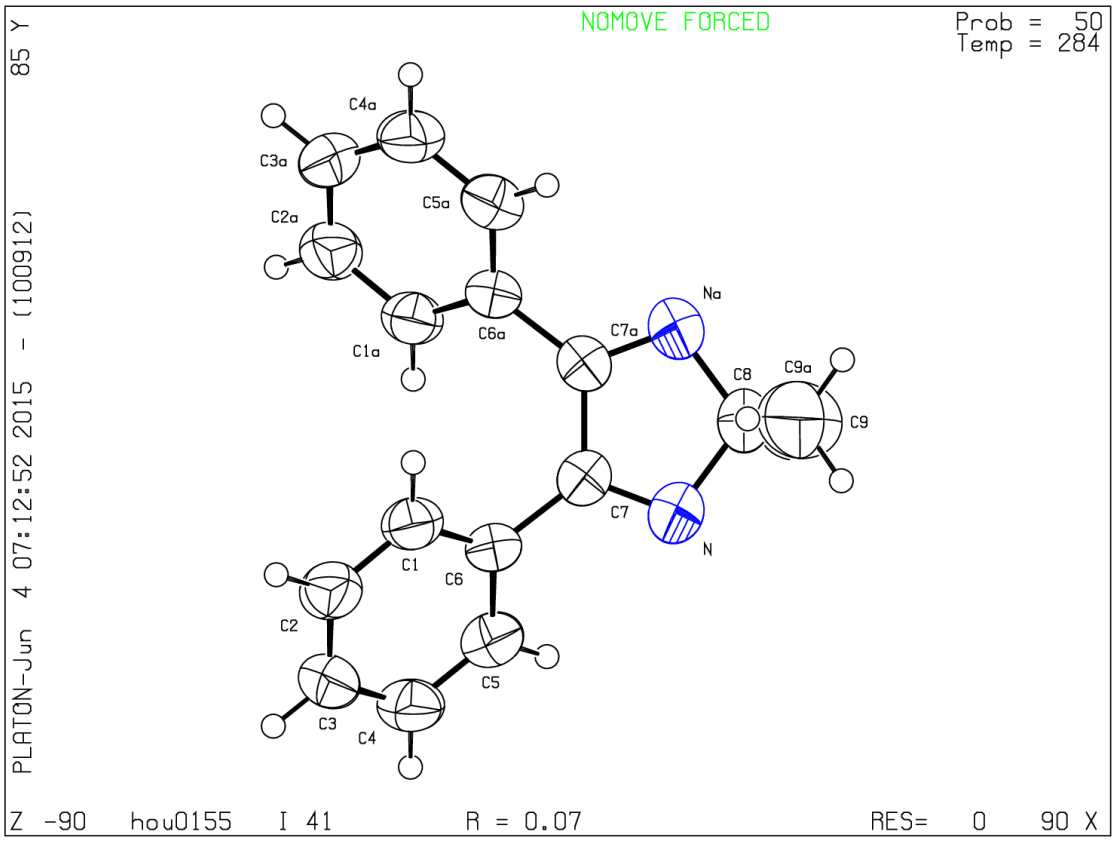


Table 1. Crystal data and structure refinement for hou0155.

Identification code	hou0155	
Empirical formula	C17 H16 N2	
Formula weight	248.32	
Temperature	284(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I 41	
Unit cell dimensions	a = 10.6396(6) Å	α= 90°.
	b = 10.6396(6) Å	β= 90°.
	c = 13.8377(8) Å	γ = 90°.
Volume	1566.44(15) $Å^3$	
Z	4	
Density (calculated)	1.053 Mg/m^3	
Absorption coefficient	0.062 mm^{-1}	
F(000)	528	
Crystal size	0.48 x 0.28 x 0.24 mm^3	
Theta range for data collection	3.83 to 26.29°.	
Index ranges	-13<=h<=13, -13<=k<=13, -17<=l<=17	
Reflections collected	10603	
Independent reflections	1604 [R(int) = 0.0242]	
Completeness to theta = 26.29°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9852 and 0.9706	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1604 / 1 / 88	
Goodness-of-fit on F^2	1.066	
Final R indices [I>2sigma(I)]	R1 = 0.0689, wR2 = 0.2026	
R indices (all data)	R1 = 0.0763, wR2 = 0.2158	
Absolute structure parameter	1(8)	
Extinction coefficient	0.015(6)	
Largest diff. peak and hole	0.461 and -0.149 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for hou0155. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N	9930(4)	3879(3)	-639(2)	101(1)
C(1)	10791(3)	3668(2)	1833(2)	62(1)
C(2)	10822(3)	2844(3)	2597(2)	71(1)
C(3)	10048(4)	1808(3)	2612(2)	75(1)
C(4)	9251(3)	1591(3)	1848(3)	74(1)
C(5)	9203(3)	2399(3)	1084(2)	67(1)
C(6)	9966(3)	3452(2)	1073(2)	57(1)
C(7)	9953(3)	4304(3)	223(2)	70(1)
C(8)	10000	5000	-1275(4)	123(3)
C(9)	8605(11)	5121(6)	-1797(4)	215(5)

Table 3. Bond lengths [Å] and angles [°] for hou0155.

N-C(7)	1.276(3)
N-C(8)	1.484(4)
C(1)-C(2)	1.373(4)
C(1)-C(6)	1.389(4)
C(1)-H(1A)	0.9300
C(2)-C(3)	1.376(5)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.376(5)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.363(5)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.384(4)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.485(4)
C(7)-C(7)#1	1.484(6)
C(8)-N#1	1.484(4)
C(8)-C(9)	1.656(9)
C(8)-C(9)#1	1.656(9)
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600

C(7)-N-C(8)	105.6(3)
C(2)-C(1)-C(6)	119.5(2)
C(2)-C(1)-H(1A)	120.2
C(6)-C(1)-H(1A)	120.2
C(1)-C(2)-C(3)	120.6(3)
C(1)-C(2)-H(2A)	119.7
C(3)-C(2)-H(2A)	119.7
C(2)-C(3)-C(4)	119.4(3)
C(2)-C(3)-H(3A)	120.3
C(4)-C(3)-H(3A)	120.3
C(5)-C(4)-C(3)	120.9(3)
C(5)-C(4)-H(4A)	119.6

C(3)-C(4)-H(4A)	119.6
C(4)-C(5)-C(6)	119.9(3)
C(4)-C(5)-H(5A)	120.1
C(6)-C(5)-H(5A)	120.1
C(5)-C(6)-C(1)	119.7(3)
C(5)-C(6)-C(7)	119.9(3)
C(1)-C(6)-C(7)	120.3(2)
N-C(7)-C(6)	121.6(3)
N-C(7)-C(7)#1	110.78(18)
C(6)-C(7)-C(7)#1	127.47(14)
N-C(8)-N#1	107.3(4)
N-C(8)-C(9)	106.0(3)
N#1-C(8)-C(9)	104.0(3)
N-C(8)-C(9)#1	104.0(3)
N#1-C(8)-C(9)#1	106.0(3)
C(9)-C(8)-C(9)#1	128.3(7)
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,z+0

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for hou0155. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N	184(4)	65(2)	55(1)	-6(1)	-2(2)	4(2)
C(1)	71(2)	48(1)	68(2)	-4(1)	-6(1)	-3(1)
C(2)	87(2)	57(1)	70(2)	-3(1)	-15(2)	9(1)
C(3)	107(2)	52(1)	67(2)	8(1)	7(2)	4(1)
C(4)	92(2)	51(1)	81(2)	-1(1)	9(2)	-16(1)
C(5)	78(2)	55(1)	69(2)	-9(1)	-1(1)	-6(1)
C(6)	75(2)	40(1)	56(1)	-3(1)	1(1)	3(1)
C(7)	104(2)	54(2)	52(2)	-4(1)	-3(2)	1(1)
C(8)	248(9)	70(3)	49(2)	0	0	5(4)
C(9)	414(15)	105(4)	127(4)	8(3)	-167(7)	-16(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for hou0155.

	x	y	z	U(eq)
H(1A)	11318	4365	1825	75
H(2A)	11371	2988	3108	85
H(3A)	10063	1259	3136	90
H(4A)	8738	883	1851	89
H(5A)	8659	2243	572	81
H(9A)	7965	5167	-1309	323
H(9B)	8460	4399	-2197	323
H(9C)	8580	5867	-2186	323